	PDB annotation	TYROSINE-PROTEIN KINASE	SIGNAL TRANSDUCTION PROTEIN	SIGNAL TRANSDUCTION PROTEIN	SIGNALING PROTEIN	DAPP1, PHISH, BAM32; PLECKSTRIN, 3-	PHOSPHOINOSITIDES,	INOSITOL	TETRAKISPHOSPHATE 2	SIGNAL TRANSDUCTION	PROTEIN, ADAPTOR	PROTEIN	SIGNALING PROTEIN	DAPP1, PHISH, BAM32;	PLECKSTRIN, 3-	PHOSPHOINOSITIDES,	INOSITOL	TETRAKISPHOSPHATE 2	SIGNAL TRANSDUCTION	PROTEIN, ADAPTOR	PROTEIN					
	Compound		BETA-SPECTRIN; 1BTN 4 CHAIN: NULL; 1BTN 5	BETA-SPECTRIN; 1BTN 4 CHAIN: NULL; 1BTN 5	DUAL ADAPTOR OF	PHOSPHOTYROSINE AND 3- CHAIN: A;						TO COMPANY ATTACK	DUAL ADAPTOR OF	PHOSPHOTYROSINE AND 3-	CHAIN: A;							PHOSPHORYLATION PLECKSTRIN (N-TERMINAL	PLECKSTRIN HOMOLOGY	DOMAIN) MUTANT 1PLS 3 WITH	LEU GLU (HIS)6 ADDED TO THE	C TERMINUS 1PLS 4 (INS(G105- LEHHHHHH) (NMR. 25
Table 5	SEQ FOLD score																					,				
Tal	PMF score		60.0	-0.01	08.0							7.0	D. /4									0.35		***		
	Verify score		-0.14	0.03	0.64				•			100	0.37									0.34				
	Psi Blast		4.4e-11	1.2e-08	3.4e-20							00 7 7	3.4e-20									1.1e-18				
	END		113	112	112							110	711									123				
	START AA		10	8	8	*****						0	•									5				
	CHAIN ID				A								τ.													
	PDB ID		1btn	1btn	1fao							140	1100									lpls				
	SEQ NO EQ		1419	1419	1419							1410	1417								-	1419				_

	PDB annotation								SIGNAL TRANSDUCTION	IRS-1; BETA-SANDWHICH,	CICNAL TRANSPOCITOR	MO 1 DEET CANDIMICAL	IKS-1; BETA-SANDWHICH, SIGNAL TRANSDUCTION	KINASE KINASE, SIGNAL	TRANSDUCTION,	CALCIUM/CALMODULIN	KINASE KINASE, SIGNAL	TRANSDUCTION, CALCITM/CALMODITIN	TRANSFERASE	TRANSFERASE,	SERINE/THREONINE-	PROTEIN KINASE, CASEIN	KINASE, 2 SER/THR KINASE			
	Compound		STRUCTURES) 1PLS 5	PHOSPHORYLATION PLECKSTRIN (N-TERMINAL	PLECKSTRIN HOMOLOGY	LEU GLU (HIS)6 ADDED TO THE	C TERMINUS 1PLS 4 (INS(G105- LEHHHHHHH)) (NMR, 25	STRUCTURES) 1PLS 5	INSULIN RECEPTOR	SUBSTRATE 1; CHAIN: A, B;	INSTIT IN DECEDIOD	CITIESTE ATTE 1. CITABLE A DE	SUBSIKAIE I; CHAIN: A, B;	CALCIUM/CALMODULIN-	DEPENDENT PROTEIN KINASE;	CHAIN: NOLL;	CALCIUM/CALMODULIN-	DEPENDENT PROTEIN KINASE; CHAIN: NULL:	PROTEIN KINASE CK2/ALPHA-	SUBUNIT; CHAIN: NULL;				TRANSFERASE(PHOSPHOTRANS FERASE) \$C-/AMP\$-DEPENDENT	PROTEIN KINASE (E.C.2.7.1.37)	OUT TOUTED CIVITAL (SALADE)
Table 5	SEQ	FOLD																								
Ta	PMF	score		69.0					0.90		0.30)		0.31		1	0.77		0.84					0.10		
	Verify	score		0.36					0.40		0.06	9		-0.47			0.65		06.0					-0.19		
	Psi	Blast		3.4e-12					1e-16		6 60-73			1.3e-05		1	5.1e-78		6.8e-37					1.1e-06		
	END	AA		118					114		151			203		0,1	510		511					198		
	START	AA		7					5		5	•		118		0.00	7/7		279					118		
	CHAIN	3							A		A													ш		
	PDB	a		1pls					1qqg		1000	OLT.		1a06		,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	1a06		1a60					lapm		
	SEQ	⊇ <u>ö</u>		1419					1419		1419			1420		007.	1470		1420					1420		

	PDB annotation																														PROTEIN KINASE CDK2;	PROTEIN KINASE, CELL
	Compound			SUBUNIT) "ALPHA" ISOENZYME MUTANT WITH SER 139 1APM 4	REPLACED BY ALA (/S139A\$)	COMPLEX WITH THE PEPTIDE	1APM 5 INHIBITOR PKI(5-24)	AND THE DETERGENT MEGA-8	IAPM 6	I KANSFEKASE(PHOSPHOTRANS	PECASE) &C-/AMP\$-DEPENDENT	(\$C/APK\$) 1APM 3 (CATALVIT)	SI IBI INITA "AI DHA" ISOENIAAA	MUTANT WITH SER 139 1APM 4	REPLACED BY ALA (/S139A\$)	COMPLEX WITH THE PEPTIDE	1APM 5 INHIBITOR PKI(5-24)	AND THE DETERGENT MEGA-8	1APM 6	TRANSFERASE(PHOSPHOTRANS	FERASE) \$C-/AMP\$-DEPENDENT	PROTEIN KINASE (E.C.2.7.1.37)	(\$C/APK\$) 1APM 3 (CATALYTIC	SUBUNIT) "ALPHA" ISOENZYME	MUTANT WITH SER 139 1APM 4	REPLACED BY ALA (/S139A\$)	COMPLEX WITH THE PEPTIDE	1APM 5 INHIBITOR PKI(5-24)	AND THE DETERGENT MEGA-8	1APM 6	CYCLIN-DEPENDENT PROTEIN	KINASE 2; CHAIN: NULL;
Table 5	SEQ	FOLD	score							88.91													•									
Ta	PMF	score																		1.00											0.93	
	Verify	score																		09.0											69.0	
	Psi	Blast								>										0											le-51	
	END	AA							610	210										513				-							511	
	START	AA							212	212										248				•							278	
	CHAIN								Ĺ	<u> </u>		•	-						1	т) 												
	PDB								1 onm	1 apm									\dashv	lapm										,	laql	
	SEQ) 							1/120	0751									00,	1420											1420	

	PDB annotation	CYCLE, PHOSPHORYLATION, STAUROSPORINE, 2 CELL DIVISION, MITOSIS, INHIBITION	COMPLEX (KINASE/INHIBITOR) CDK6; P19INK4D; CYCLIN DEPENDENT KINASE, CYCLIN DEPENDENT KINASE INHIBITORY 2 PROTEIN, CDK, INK4, CELL CYCLE, COMPLEX (KINASE/INHIBITOR) HEADER HELIX	COMPLEX (KINASE/INHIBITOR) CDK6; P19INK4D; CYCLIN DEPENDENT KINASE, CYCLIN DEPENDENT KINASE INHIBITORY 2 PROTEIN, CDK, INK4, CELL CYCLE, COMPLEX (KINASE/INHIBITOR) HEADER HELIX	COMPLEX (INHIBITOR PROTEIN/KINASE) INHIBITOR PROTEIN, CYCLIN-DEPENDENT KINASE, CELL CYCLE 2 CONTROL, ALPHA/BETA,
	Compound		CYCLIN-DEPENDENT KINASE 6; CHAIN: A, C; CYCLIN- DEPENDENT KINASE INHIBITOR; CHAIN: B, D;	CYCLIN-DEPENDENT KINASE 6; CHAIN: A, C; CYCLIN- DEPENDENT KINASE INHIBITOR; CHAIN: B, D;	CYCLIN-DEPENDENT KINASE 6; CHAIN: A; P19INK4D; CHAIN: B;
Table 5	SEQ FOLD	2003	62.61		
Та	PMF			0.36	0.57
	Verify score			0.37	0.55
	Psi Blast		3.4e-44	3.4e-44	3.4e-45
	END		518	509	511
	START AA		279	281	281
	CHAIN		А	A	A
	PDB U		1bi8	15i8	1blx
	(A) (B) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A		1420	1420	1420

	PDB annotation		COMPLEX (INHIBITOR PROTEIN/KINASE)	TRANSFERASE STRESS- ACTIVATED PROTEIN KINASE-3, ERK6, ERK5; P38- GAMMA, GAMMA, PHOSPHORYLATION, MAP KINASE		,			
	Compound			PHOSPHORYLATED MAP KINASE P38-GAMMA; CHAIN: A, B;	PHOSPHOTRANSFERASE CAMP- DEPENDENT PROTEIN KINASE CATALYTIC SUBUNIT 1CMK 3 (E.C.2.7.1.37) 1CMK 4	PHOSPHOTRANSFERASE CAMP- DEPENDENT PROTEIN KINASE CATALYTIC SUBUNIT 1CMK 3 (E.C.2.7.1.37) 1CMK 4	TRANSFERASE(PHOSPHOTRANS FERASE) CAMP-DEPENDENT PROTEIN KINASE (E.C.2.7.1.37) (CAPK) 1CTP 3 (CATALYTIC SUBUNIT) 1CTP 4	TRANSFERASE(PHOSPHOTRANS FERASE) CAMP-DEPENDENT PROTEIN KINASE (E.C.2.7.1.37) (CAPK) 1CTP 3 (CATALYTIC SUBUNIT) 1CTP 4	TRANSFERASE(PHOSPHOTRANS FERASE) CAMP-DEPENDENT PROTEIN KINASE (E.C.2.7.1.37) (CAPK) 1CTP 3 (CATALYTIC SUBUNIT) 1CTP 4
Table 5	SEQ	FOLD			93.62			97.24	
Tak	PMF	score		0.71		0.98	0.37		1.00
	Verify	score		0.61		0.63	-0.47		0.59
	Psi	Blast		1.5e-41	0	0	8.8e-07	0	0
	END	AA		511	518	513	198	518	513
	START	AA		295	208	243	118	210	248
	CHAIN	А		¥	ш	E	ы	ਬ	lд
	PDB	А		1cm8	1cmk	1cmk	1ctp	1ctp	1ctp
	SEQ	A Š		1420	1420	1420	1420	1420	1420

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	PDB annotation		TRANSFERASE KINASE DOMAIN, AUTOINHIBITORY FRAGMENT, HOMODIMER	PROTEIN KINASE CDK2; TRANSFERASE, SERINE/THREONINE PROTEIN KINASE, ATP- BINDING, 2 CELL CYCLE, CELL DIVISION, MITOSIS, PHOSPHORYLATION	PROTEIN KINASE CDK2; TRANSFERASE, SERINE/THREONINE PROTEIN KINASE, ATP- BINDING, 2 CELL CYCLE, CELL DIVISION, MITOSIS, PHOSPHORYLATION	SERINE/THREONINE- PROTEIN KINASE CSBP, RK, P38; PROTEIN SER/THR- KINASE, SERINE/THREONINE- PROTEIN KINASE	COMPLEX (TRANSFERASE/SUBSTRATE) TYROSINE KINASE, SIGNAL TRANSDUCTION, PHOSPHOTRANSFERASE, 2 COMPLEX (KINASE/PEPTIDE
Table 5	Compound		SERINE/THREONINE-PROTEIN KINASE PAK-ALPHA; CHAIN: A, B; SERINE/THREONINE- PROTEIN KINASE PAK-ALPHA; CHAIN: C, D;	HUMAN CYCLIN-DEPENDENT KINASE 2; CHAIN: NULL;	HUMAN CYCLIN-DEPENDENT KINASE 2; CHAIN: NULL;	P38 MAP KINASE; CHAIN: NULL;	NSULIN RECEPTOR; CHAIN: A; PEPTIDE SUBSTRATE; CHAIN: B;
	SEQ	FOLD		62.10			75.00
Tak	PMF	score	0.86		0.98	0.53	
	Verify	score	0.73		0.49	0.32	
	Psi	Blast	1.7e-52	3.4e-53	3.4e-53	1e-36	5.1e-26
	END	AA	509	517	511	515	518
	START	ΑA	279	247	278	278	230
	CHAIN		U				A
	PDB	<u> </u>	1f3m	lhcl	1hcl	lian	lir3
	SEQ	A È	1420	1420	1420	1420	1420

	PDB annotation		SUBSTRATE/ATP ANALOG), ENZYME, 3 COMPLEX (TRANSFERASE/SUBSTRATE)	TRANSFERASE JNK3; TRANSFERASE, JNK3 MAP KINASE, SERINE/THREONINE PROTEIN 2 KINASE	KINASE KINASE, TWITCHIN, INTRASTERIC REGULATION	KINASE KINASE, TWITCHIN, INTRASTERIC REGULATION	TRANSFERASE MITOGEN ACTIVATED PROTEIN KINASE; TRANSFERASE, MAP KINASE, SERINE/THREONINE-	KINASE RABBIT MUSCLE PHOSPHORYLASE KINASE; GLYCOGEN METABOLISM, TRANSFERASE, SERINE/THREONINE- PROTEIN, 2 KINASE, ATP- BINDING, CALMODULIN- BINDING	KINASE RABBIT MUSCLE PHOSPHORYLASE KINASE; GLYCOGEN METABOLISM, TRANSFERASE,
Table 5	Compound			C-JUN N-TERMINAL KINASE; CHAIN: NULL;	TWITCHIN; CHAIN: NULL;	TWITCHIN; CHAIN: A, B;	MAP KINASE P38; CHAIN: NULL;	PHOSPHORYLASE KINASE; CHAIN: NULL;	PHOSPHORYLASE KINASE; CHAIN: NULL;
	SEQ FOLD	score							75.54
Tal	PMF			0.94	0.48	0.87	0.43	0.03	
	Verify score			9.02	19.0	89.0	0.57	-0.39	
	Psi Blast			1.7e-40	5.1e-62	1.2e-62	5.1e-43	6.6e-06	5.1e-73
	END	1		508	507	510	515	203	512
	START	1		278	267	273	278	118	250
	CHAIN	1				A			
	PDB			1jnk	1koa	1kob	1p38	1phk	1 phk
	SEQ	e ë		1420	1420	1420	1420	1420	1420

	PDB annotation	SERINE/THREONINE- PROTEIN, 2 KINASE, ATP- BINDING, CALMODULIN- BINDING	KINASE RABBIT MUSCLE PHOSPHORYLASE KINASE; GLYCOGEN METABOLISM, TRANSFERASE, SERINE/THREONINE- PROTEIN, 2 KINASE, ATP- BINDING, CALMODULIN- BINDING	TRANSFERASE MAP KINASE, SERINE/THREONINE PROTEIN KINASE, TRANSFERASE	SERINE KINASE SERINE KINASE, TITIN, MUSCLE, AUTOINHIBITION	TRANSFERASE MITOGEN ACTIVATED PROTEIN KINASE, MAP 2, ERK2; TRANSFERASE, SERINE/THREONINE- PROTEIN KINASE, MAP KINASE, 2 ERK2	POTASSIUM CHANNELS POTASSIUM CHANNELS, TETRAMERIZATION
	Compound		PHOSPHORYLASE KINASE; CHAIN: NULL;	ERK2; CHAIN: NUIL;	TITIN; CHAIN: A, B;	EXTRACELLULAR REGULATED KINASE 2; CHAIN: NULL;	POTASSIUM CHANNEL KV1.1; CHAIN: NULL;
Table 5	SEQ FOLD score						
Tal	PMF score		0.94	0.43	0.49	0.48	0.98
	Verify score		0.79	0.58	0.65	0.52	0.34
	Psi Blast		5.1e-73	1.5e-37	1.7e-48	6.8e-41	3.4e-26
	END AA		509	507	509	507	121
	START AA		277	291	275	281	26
	CHAIN				A		
	PDB ID		1phk	1pme	1tki	3erk	1a68
	SEQ ID	S	1420	1420	1420	1420	1427

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	PDB annotation	DOMAIN, X-RAY 2 STRUCTURE, APLYSIA KV1.1	SIGNALING PROTEIN VOLTAGE-GATED POTASSIUM CHANNEL, ASSEMBLY DOMAIN, TETRAMER	METAL TRANSPORT ION CHANNEL, OXIDOREDUCTASE, BETA SUBUNIT	SIGNALING PROTEIN VOLTAGE-GATED POTASSIUM CHANNEL, TETRAMERIZATION DOMAIN, 2 INTRACELLULAR GATE, TETRAMER	PROTON TRANSPORT POTASSIUM CHANNELS, TETRAMERIZATION DOMAIN, X-RAY STRUCTURE, 2 APLYSIA KV1.1, PROTON TRANSPORT	POTASSIUM CHANNEL POTASSIUM CHANNEL, TETRAMERIZATION DOMAIN, MOLECULAR 2 RECOGNITION, ZINC- BINDING
	Compound		KV1.2 VOLTAGE-GATED POTASSIUM CHANNEL; CHAIN: A, B, C, D, E, F, G, H;	KV BETA2 PROTEIN; CHAIN: A; POTASSIUM CHANNEL KV1.1; CHAIN: E;	KV1.2 VOLTAGE-GATED POTASSIUM CHANNEL; CHAIN: A, B, C, D;	POTASSIUM CHANNEL KV1.1; CHAIN: A;	POTASSIUM CHANNEL PROTEIN SHAW; CHAIN: NULL;
Table 5	SEQ FOLD	2006					
Tab	PMF		0.75	0.80	0.82	0.94	66:0
	Verify score		0.28	0.53	0.26	0.34	99.0
	Psi Blast		5.1e-25	1e-25	6.8e-27	1.7e-26	1.5e-29
	END		121	123	133	134	136
	START AA		26	26	26	26	27
	CHAIN		Ą	ET .	<	A	
	PDB		1dsx	1exb	1qdv	1114	3kvt
	SEQ	.; O N	1427	1427	1427	1427	1427

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	COGENE,	AT ELL GENE,	r IPTION ETA1;	TION NA-	<u>_</u>	TOR	NOIT	[A1;	TION IA-	Ļ	. ^	TOR	TION	1٠	TION	[A-	
	ANTI-ONCOGENE CELL CYCLE, ANTI-ONCOGENE,	REPEAT, ANK REPEAT ANTI-ONCOGENE CELL CYCLE, ANTI-ONCOGENE,	REPEAT, ANK REPEAT COMPLEX (TRANSCRIPTION REGULATION/DNA) GABPALPHA: GABPBETA1;	COMPLEX (TRANSCRIPTION REGULATION/DNA), DNA-BINDING, 2 NUCLEAR	PROTEIN, ETS DOMAIN, ANKYRIN REPEATS,	TRANSCRIPTION 3 FACTOR	COMPLEX (TRANSCRIPTION REGIT ATTON/DNA)	GABPALPHA; GABPBETA1;	COMPLEX (TRANSCRIPTION	BINDING, 2 NUCLEAR	PROTEIN, ETS DOMAIN,	ANKYRIN REPEATS, TP ANSCRIPTION 3 FACTOR	COMPLEX (TRANSCRIPTION	KEGULATION/DINA) CAPPAT PHA: GABPRETA1:	COMPLEX (TRANSCRIPTION	REGULATION/DNA), DNA-	DINDING, Z INOCEEMIN
	TUMOR SUPPRESSOR P16INK4A; CHAIN: NULL;	TUMOR SUPPRESSOR P16INK4A; CHAIN: NULL;	GA BINDING PROTEIN ALPHA; CHAIN: A; GA BINDING PROTEIN BETA 1: CHAIN: B:	DNA; CHAIN: D, E;			GA BINDING PROTEIN ALPHA; CHAM: A. GA BINDING	PROTEIN BETA 1; CHAIN: B;	DNA; CHAIN: D, E;				GA BINDING PROTEIN ALPHA;	CHAIN: A; GA BINDING	DNA; CHAIN: D, E;		
SCOTE	61.39																
score		0.92	1.00				1.00						1.00				
score		0.44	0.88				0.54						0.43				
Blast	6e-25	1.2e-30	1.2e-39				5.1e-37						5.1e-36				
AA	284	160	164				262				,		291				
AA	134	31	10				116						149				
a			В		<u>". </u>		В						В				
A	1a5e	1a5e	lawc				1awc						1awc				
日党	1430	1430	1430				1430						1430				
0.000 0.000 1000 1000	ID ID AA AA Diast score score	1a5e 134 284 6e-25 CHAIN: NULL;	D	10 11	134 284 6e-25 61.39 TUMOR SUPPRESSOR PI6INK4A; CHAIN: NULL; CHAIN: A; GA BINDING PROTEIN ALPHA; CHAIN: A; GA BINDING PROTEIN BETA 1; CHAIN: B; DNA; CHAIN: D, E; DNA; CHAIN: D, E; CHAIN: D, E;	126 134 284 6e-25 61.39 TUMOR SUPPRESSOR P16INK4A; CHAIN: NULL; 145e 160 1.2e-30 0.44 0.92 TUMOR SUPPRESSOR P16INK4A; 12e-39 0.88 1.00 GA BINDING PROTEIN ALPHA; CHAIN: A; GA BINDING PROTEIN B; DNA; CHAIN: D, E; DNA; CHAIN: D, E; CHAIN:	14	126 126-36 1.26-37 1.26-39 1.26-39 1.00 1.26-39 1.00 1.26-39 1.26-39 1.00 1.26-39 1.26-39 1.00 1.26-39 1.26	136 134 284 6e-25 61.39 TUMOR SUPPRESSOR PIGINKAA; A	14	134 284 6e-25 61.39 TUMOR SUPPRESSOR P16INK4A; A CHAIN: NULL; B 116 262 5.1e-37 0.54 1.00 CHAIN: D, E; DNA; CHAIN: D	134 284 66-25 61.39 TUMOR SUPPRESSOR PIGNK4A; A character 134 284 66-25 61.39 TUMOR SUPPRESSOR PIGNK4A; A character 134 284 66-25 61.39 TUMOR SUPPRESSOR PIGNK4A; A character 134 160 1.26-30 0.44 0.92 TUMOR SUPPRESSOR PIGNK4A; A character 134 134 136 1.26-39 0.88 1.00 CHAIN: NULL; A character 134 136	134 284 66-25 61.39 TUMOR SUPPRESSOR PIGNK4A; A CHAIN: NULL; B 160 1.26-30 0.44 0.92 TUMOR SUPPRESSOR PIGNK4A; A CHAIN: NULL; B 10 164 1.26-39 0.88 1.00 CHAIN: NULL; B 1.00 CHAIN: B; B 1.00 CHAIN: B; B 1.00 CHAIN: B; B 1.00 CHAIN: A; GA BINDING PROTEIN ALPHA; B 1.00 CHAIN: A; GA BINDING PROTEIN B; B 1.00 CHAIN: A; GA BINDING PROTEIN B; B 1.00 CHAIN: B; B 1.00 CHAIN: B; B 1.00 CHAIN: B; B 1.00 CHAIN: D, E; B 1.00	134 284 6e-25 61.39 TUMOR SUPPRESSOR PIGINKA4; 145e 134 284 6e-25 61.39 TUMOR SUPPRESSOR PIGINKA4; 145e 12e-30 0.44 0.92 TUMOR SUPPRESSOR PIGINKA4; 145e 1.2e-39 0.88 1.00 GA BINDING PROTEIN ALPHA; 145e 116 262 5.1e-37 0.54 1.00 GA BINDING PROTEIN ALPHA; 145e 149 291 5.1e-36 0.43 1.00 GA BINDING PROTEIN ALPHA; 145e 149 291 5.1e-36 0.43 1.00 GA BINDING PROTEIN ALPHA; 145e 145	134 284 66-25 61.39 TUMOR SUPPRESSOR PIGINK4A; CHAIN: NULL; CHAIN: A; CHAIN: A; CHAIN: B; CHAIN: B; CHAIN: A; CHAIN: B; CHAIN: CHAIN: CHAIN: B; CHAIN: CHAIN: CHAIN: B; CHAIN: CHAIN: CHAIN: B; CHAIN:	134 284 66-25 61.39 TUMOR SUPPRESSOR PIGINKAA; A change 134 284 66-25 61.39 TUMOR SUPPRESSOR PIGINKAA; A change 134 160 1.26-30 0.44 0.92 TUMOR SUPPRESSOR PIGINKAA; A change 134 160 1.26-39 0.88 1.00 CHAIN: NULL; CHAIN: B; DIVA; CHAIN: D; E; DIVA; CHAIN: D; C	134 284 66-25 61.39 TUMOR SUPPRESSOR PIGINK44; CHAIN: NULL; CHAIN:

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	PDB annotation	PROTEIN, ETS DOMAIN, ANKYRIN REPEATS, TRANSCRIPTION 3 FACTOR	COMPLEX (TRANSCRIPTION REGULATION/DNA) GABPALPHA; GABPBETA1; COMPLEX (TRANSCRIPTION REGULATION/DNA), DNA- BINDING, 2 NUCLEAR PROTEIN, ETS DOMAIN,	TRANSCRIPTION 3 FACTOR	COMPLEX (TRANSCRIPTION REGULATION/DNA)	GABPALPHA; GABPBETA1;	COMPLEX (TRANSCRIPTION	REGULATION/DNA), DNA-	BINDING, 2 NUCLEAR	PROTEIN, ETS DOMAIN,	ANK YKIN KEPEA I S, TRANSCRIPTION 3 FACTOR	COMPLEX (TRANSCRIPTION	REGULATION/DNA)	GABPALPHA; GABPBETA1;	COMPLEX (TRANSCRIPTION	REGULATION/DNA), DNA-	BINDING, 2 NUCLEAR	PROTEIN, ETS DOMAIN,	ANKYRIN REPEATS,	COMPLEY (TRANSCRIPTION	COM PEA (110m) COM 110m
	Compound		GA BINDING PROTEIN ALPHA; CHAIN: A; GA BINDING PROTEIN BETA 1; CHAIN: B; DNA; CHAIN: D, E;		GA BINDING PROTEIN ALPHA; CHAIN: A: GA BINDING	PROTEIN BETA 1; CHAIN: B;	DNA; CHAIN: D, E;					GA BINDING PROTEIN ALPHA;	CHAIN: A; GA BINDING	PROTEIN BETA 1; CHAIN: B;	DNA; CHAIN: D, E;					GA BINDING BROTEIN AI BHA:	OR BINDAINO I NO I DIIN DELI 1171,
Table 5	SEQ FOLD score																			9K 12	00.17
Tal	PMF		1.00		1.00							1.00									
	Verify score		0.91		0.70							96.0									
	Psi Blast		3.4e-34		8.5e-30					-		1.2e-39								150 41	1.25-41
	END		164		299							196								100	170
	START AA		16		182							46								71	40
	CHAIN ID		В		В							В								۲	Б
	PDB ID		lawc		lawc							lawc									Iawc
	SEQ EQ		1430		1430							1430								1420	1430

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	PDB annotation		REGULATION/DNA) GABPALPHA; GABPBETA1; COMPI EX /TRANSCRIPTION	REGULATION/DNA), DNA-	BINDING, 2 NUCLEAR	PROTEIN, ETS DOMAIN,	ANKYRIN REPEATS, TRANSCRIPTION 3 FACTOR	COMPLEX (TRANSCRIPTION	REGULATION/DNA)	GABPALPHA; GABPBETA1;	COMPLEX (TRANSCRIPTION	REGULATION/DNA), DNA-	BINDING, 2 NUCLEAR	PROTEIN, EIS DOMAIN,	ANKYKIN KEPEATS,	I KANSCKIP I ION 3 FACTOR	COMPLEX (TRANSCRIPTION	REGULATION/DNA)	GABPALPHA; GABPBETA1;	COMPLEX (TRANSCRIPTION	REGULATION/DNA), DNA-	BINDING, 2 NUCLEAR	PROTEIN, ETS DOMAIN,	ANKYRIN REPEATS,	TRANSCRIPTION 3 FACTOR	COMPLEX (TRANSCRIPTION	REGULATION/DNA)	GABPALPHA; GABPBETA1;	COMPLEX (TRANSCRIPTION REGULATION/DNA), DNA-	
			100													-		_	_	_										
	Compound		CHAIN: A; GA BINDING PROTEIN BETA 1; CHAIN: B;	DINA, CITAIN. D, E,				GA BINDING PROTEIN ALPHA;	CHAIN: A; GA BINDING	PROTEIN BETA 1; CHAIN: B;	DNA; CHAIN: D, E;						GA BINDING PROTEIN ALPHA;	CHAIN: A; GA BINDING	PROTEIN BETA 1; CHAIN: B;	DNA; CHAIN: D, E;						GA BINDING PROTEIN ALPHA;	CHAIN: A; GA BINDING	PROTEIN BETA 1; CHAIN: B;	DNA; CHAIN: D, E;	
Table 5	SEQ	FOLD																												
Ta	PMF	score						1.00									1.00									1.00				
	Verify	score						1.09			-						0.48									1.00				
	Psi	Blast						1.5e-39									1.2e-30									1.5e-41				
	END	AA						197		•							131									230				
	START	AA						50									8								-	83				
	CHAIN	А						В									В									В				
	PDB	А						1awc									lawc									lawc				
	SEQ	日 <u>ஜ</u>						1430									1430									1430				

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	PDB annotation	BINDING, 2 NUCLEAR PROTEIN, ETS DOMAIN, ANKYRIN REPEATS, TRANSCRIPTION 3 FACTOR	TUMOR SUPPRESSOR, TUMOR SUPPRESSOR, CDK4/6 INHIBITOR, ANKYRIN MOTIF	TUMOR SUPPRESSOR, TUMOR SUPPRESSOR, CDK4/6 INHIBITOR, ANKYRIN MOTIF	TUMOR SUPPRESSOR TUMOR SUPPRESSOR, CDK4/6 INHIBITOR, ANKYRIN MOTIF	TUMOR SUPPRESSOR TUMOR SUPPRESSOR, CDK4/6 INHIBITOR, ANKYRIN MOTIF	TUMOR SUPPRESSOR TUMOR SUPPRESSOR, CDK4/6 INHIBITOR, ANKYRIN MOTIF	TUMOR SUPPRESSOR TUMOR SUPPRESSOR, CDK4/6 INHIBITOR, ANKYRIN MOTIF	TUMOR SUPPRESSOR TUMOR SUPPRESSOR, CDK4/6 INHIBITOR,
		PRO ANK TRA	TUN TUN CDIK	AUT TUN CDX	A COUNTY	A CD II	\$ 5 5 5 K	A G T T	229
	Compound		P19INK4D CDK4/6 INHIBITOR; CHAIN: NULL;	P19INK4D CDK4/6 INHIBITOR; CHAIN: NULL;	P19INK4D CDK4/6 INHIBITOR; CHAIN: NULL;	P19INK4D CDK4/6 INHIBITOR; CHAIN: NULL;	P19INK4D CDK4/6 INHIBITOR; CHAIN: NULL;	P19INK4D CDK4/6 INHIBITOR; CHAIN: NULL;	P19INK4D CDK4/6 INHIBITOR; CHAIN: NULL;
Table 5	SEQ FOLD		82.84						
Tab	PMF			1.00	1.00	1.00	1.00	1.00	1.00
	Verify score			0.67	0.49	0.53	0.84	0.78	0.86
	Psi Blast		2.4e-40	4.8e-34	3.4e-28	2.4e-40	1.4e-29	7.2e-38	3.4e-33
	END		167	264	262	165	291	198	197
	START		11	112	119	15	152	46	53
	CHAIN								
	PDB		1bd8	1bd8	1bd8	15d8	1bd8	1bd8	1bd8
	SEQ	C	1430	1430	1430	1430	1430	1430	1430

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	PDB annotation	ANKYRIN MOTIF	COMPLEX (KINASE/ANTI- ONCOGENE) CDK6;	P16INK4A, MTS1; CYCLIN	DEPENDENT KINASE,	CI CLIN DEFENDENT KINASE INHIBITORY 2	PROTEIN, CDK, INK4, CELL	CYCLE, MULTIPLE TUMOR	SUPPRESSOR, 3 MTS1,	COMPLEX (KINASE/ANTI-	ONCOGENE) HEADER	COMPLEX (INHIBITOR	PROTEIN/KINASE)	INHIBITOR PROTEIN,	CYCLIN-DEPENDENT	KINASE, CELL CYCLE 2	CONTROL, ALPHA/BETA,	COMPLEX (INHIBITOR	PROTEIN/KINASE)	COMPLEX (INHIBITOR	PROTEIN/KINASE)	INHIBITOR PROTEIN,	CYCLIN-DEPENDENT	KINASE, CELL CYCLE 2	CONTROL, ALPHA/BETA,	COMPLEX (INHIBITOR	PROTEIN/KINASE)	COMPLEX (INHIBITOR	PROTEIN FINANSE) INHIBITOR PROTEIN,
	Compound		CYCLIN-DEPENDENT KINASE 6; CHAIN: A; MULTIPLE TUMOR	SUPPRESSOR; CHAIN: B;								CYCLIN-DEPENDENT KINASE 6;	CHAIN: A; P19INK4D; CHAIN: B;							CYCLIN-DEPENDENT KINASE 6;	CHAIN: A; P19INK4D; CHAIN: B;							CYCLIN-DEPENDENT KINASE 6;	CHAIN: A; F19INK4D; CHAIN: B;
Table 5	SEQ FOLD score		59.72									80.09																	
Tab	PMF																			1.00								1.00	
	Verify score																			0.54								0.56	
	Psi Blast		2.4e-25		-							5.1e-32								6.8e-27								3.4e-29	
	END AA		267									171								262								291	!
	START		144									10							·	119								152	
	CHAIN		В									В	ı							В			***					В	
	PDB ID		1bi7									1blx								1blx	:	<u>-</u>						1blx	
	SEQ ID	5	1430		•							1430								1430	!							1430	

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	PDB annotation	CYCLIN-DEPENDENT KINASE, CELL CYCLE 2 CONTROL, ALPHA/BETA,	COMPLEX (INHIBITOR PROTEIN/KINASE)	COMPLEX (INHIBITOR PROTEIN/KINASE)	INHIBITOR PROTEIN, CYCLIN-DEPENDENT	KINASE, CELL CYCLE 2	CONTROL, ALPHA/BETA,	PROTEIN/KINASE)	HORMONE/GROWTH FACTOR P18-INK4C; CELL	CYCLE INHIBITOR,	P18INK4C, TUMOR, STIPPRESSOR CYCLIN-2	DEPENDENT KINASE.	HORMONE/GROWTH	FACTOR	HORMONE/GROWTH	FACTOR P18-INK4C; CELL	CYCLE INHIBITOR,	FISHNK4C, IUMOK,	SUPPRESSOR, CYCLIN- 2	DEPENDENT KINASE,	HORMONE/GROWTH	FACTOR	HORMONE/GROWTH FACTOR P18-INK4C; CELL
	Compound			CYCLIN-DEPENDENT KINASE 6; CHAIN: A; P19INK4D; CHAIN: B;					CYCLIN-DEPENDENT KINASE 6 INHIBITOR: CHAIN: A:						CYCLIN-DEPENDENT KINASE 6	INHIBITOR; CHAIN: A;							CYCLIN-DEPENDENT KINASE 6 INHIBITOR; CHAIN: A;
Table 5	SEQ FOLD	2000																					
Tal	PMF			1.00					1.00						1.00							-	1.00
	Verify score			0.79					29.0						0.75								0.93
	Psi Blast			5.1e-32					1.7e-32		- '				1.7e-34								8.5e-38
	END			197					267						297								202
	START AA			53					116						149								50
	CHAIN			В					A						A				J-1.				А
	PDB ID			1blx	-				1bu9					_	1bu9								1bu9
	SEQ			1430					1430						1430			_					1430

	PDB annotation	CYCLE INHIBITOR, P18INK4C, TUMOR, SUPPRESSOR, CYCLIN- 2 DEPENDENT KINASE, HORMONE/GROWTH FACTOR	HORMONE/GROWTH FACTOR P18-INK4C; CELL CYCLE INHIBITOR, P18INK4C, TUMOR, SUPPRESSOR, CYCLIN- 2 DEPENDENT KINASE, HORMONE/GROWTH FACTOR	SIGNALING PROTEIN HELIX-TURN-HELIX, ANKYRIN REPEAT	SIGNALING PROTEIN HELIX-TURN-HELIX, ANKYRIN REPEAT	CELL CYCLE INHIBITOR P18-INK4C(INK6); CELL CYCLE INHIBITOR, P18- INK4C(INK6), ANKYRIN REPEAT, 2 CDK 4/6 INHIBITOR	CELL CYCLE INHIBITOR P18-INK4C(INK6); CELL CYCLE INHIBITOR, P18- INK4C(INK6), ANKYRIN REPEAT, 2 CDK 4/6
	Compound		CYCLIN-DEPENDENT KINASE 6 INHIBITOR; CHAIN: A;	CYCLIN-DEPENDENT KINASE 4 INHIBITOR B; CHAIN: A;	CYCLIN-DEPENDENT KINASE 4 INHIBITOR B; CHAIN: A;	CYCLIN-DEPENDENT KINASE 6 INHIBITOR; CHAIN: A, B;	CYCLIN-DEPENDENT KINASE 6 INHIBITOR; CHAIN: A, B;
Table 5	SEQ FOLD score		97.65				
Tal	PMF score			0.99	0.99	1.00	1.00
	Verify score		_	0.71	0.72	0.56	0.59
	Psi Blast		8.5e-38	3.6e-36	1.1e-31	3.6e-35	8.5e-32
	END		176	169	136	168	266
	START		_∞	35	6	10	116
	CHAIN		A	A	V _	⋖	A
	PDB ID		1bu9	1d9s	1d9s	1 ihb	lihb
	SEQ ID		1430	1430	1430	1430	1430

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	PDB annotation		INHIBITOR	CELL CYCLE INHIBITOR P18-INK4C(INK6); CELL	CYCLE INHIBITOR, P18-	INK4C(INK6), ANKYRIN	REPEAT, 2 CDK 4/6	INHIBITOR	CELL CYCLE INHIBITOR P18_INK4C/INK6)· CFLI.	CYCLE INHIBITOR, P18-	INK4C(INK6), ANKYRIN	REPEAT, 2 CDK 4/6	INHIBITOR	CELL CYCLE INHIBITOR	P18-INK4C(INK6); CELL	CYCLE INHIBITOR, P18-	INK4C(INK6), ANKYRIN	REPEAT, 2 CDK 4/6	INHIBITOR	CELL CYCLE INHIBITOR	P18-INK4C(INK6); CELL	CYCLE INHIBITOR, P18-	INK4C(INK6), ANKYRIN	REPEAT, 2 CDK 4/6	INHIBITOR	TRANSCRIPTION FACTOR	P65; P50D; TRANSCRIPTION	FACTOR, IKB/NFKB	COMPLEX	TRANSCRIPTION FACTOR P65; P50D; TRANSCRIPTION	
	Compound			CYCLIN-DEPENDENT KINASE 6 INHIBITOR; CHAIN: A, B;					CYCLIN-DEPENDENT KINASE 6	INITIDITOR, CITAIN: P. D.				CYCLIN-DEPENDENT KINASE 6	INHIBITOR; CHAIN: A, B;					CYCLIN-DEPENDENT KINASE 6	INHIBITOR; CHAIN: A, B;					NF-KAPPA-B P65 SUBUNIT;	CHAIN: A; NF-KAPPA-B P50D	SUBUNIT; CHAIN: C; I-KAPPA-B-	ALPHA; CHAIN: D;	NF-KAPPA-B P65 SUBUNIT; CHAIN: A; NF-KAPPA-B P50D	
Table 5	SEQ FOLD	score		95.32					!																						
Tat	PMF								1.00					1.00						1.00						1.00				1.00	
	Verify								0.93					0.77						0.92						0.53	***			0.58	
	Psi Blast			3.4e-37					8.5e-34					3.4e-37						2.4e-35						3.4e-36				1.7e-40	
	END			168					296					201	,) 					232						181				282	
	START	, r,		12			•		149					50)					81							!			111	
	CHAIN	₹		А					A					A	4					A						٦	1			Q	
	PDB	3		1 ihb					1ihb					1.hh	OIII T					1ihb						1 ikm				1 ikm	
	SEQ			1430					1430					1430	2					1430)					1430				1430	

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	PDB annotation	FACTOR, IKB/NFKB COMPLEX	TRANSCRIPTION FACTOR P65; P50D; TRANSCRIPTION FACTOR, IKB/NFKB COMPLEX	TRANSCRIPTION FACTOR P65; P50D; TRANSCRIPTION FACTOR, IKB/NFKB COMPLEX	TRANSCRIPTION FACTOR P65; P50D; TRANSCRIPTION FACTOR, IKB/NFKB COMPLEX	ANK-REPEAT MYOTROPHIN, ACETYLATION, NMR, ANK- REPEAT	ANK-REPEAT MYOTROPHIN, ACETYLATION, NMR, ANK- REPEAT	COMPLEX (TRANSCRIPTION REG/ANK REPEAT) COMPLEX (TRANSCRIPTION REGULATION/ANK REPEAT), ANKYRIN 2 REPEAT HELIX	COMPLEX (TRANSCRIPTION REG/ANK REPEAT) COMPLEX (TRANSCRIPTION
	Compound	SUBUNIT; CHAIN: C; I-KAPPA-B-ALPHA; CHAIN: D;	NF-KAPPA-B P65 SUBUNIT; CHAIN: A; NF-KAPPA-B P50D SUBUNIT; CHAIN: C; I-KAPPA-B- ALPHA; CHAIN: D;	NF-KAPPA-B P65 SUBUNIT; CHAIN: A; NF-KAPPA-B P50D SUBUNIT; CHAIN: C; I-KAPPA-B- ALPHA; CHAIN: D;	NF-KAPPA-B P65 SUBUNIT; CHAIN: A; NF-KAPPA-B P50D SUBUNIT; CHAIN: C; I-KAPPA-B- ALPHA; CHAIN: D;	MYOTROPHIN; CHAIN: NULL	MYOTROPHIN; CHAIN: NULL	NF-KAPPA-B P65; CHAIN: A, C; NF-KAPPA-B P50; CHAIN: B, D; I- KAPPA-B-ALPHA; CHAIN: E, F;	NF-KAPPA-B P65; CHAIN: A, C; NF-KAPPA-B P50; CHAIN: B, D; I- KAPPA-B-ALPHA; CHAIN: E, F;
Table 5	SEQ FOLD score				93.44	71.55			
Tab	PMF score		1.00	1.00			0.10	1.00	1.00
	Verify score		0.53	09.0			-0.12	89.0	0.94
	Psi Blast		1.5e-33	8.5e-42	8.5e-42	3.6e-30	6e-26	1e-36	5.1e-40
	END		300	230	251	228	293	181	282
	START		144	45	45	112	147	10	109
	CHAIN		D	D	D			ш	田
	PDB ID		1 ikm	1.ikn	1 ikn	1myo	1myo	1nfi	1nfi
	SEQ NO.		1430	1430	1430	1430	1430	1430	1430

	PDB annotation	REGULATION/ANK REPEAT), ANKYRIN 2 REPEAT HELIX	COMPLEX (TRANSCRIPTION REG/ANK REPEAT) COMPLEX (TRANSCRIPTION REGULATION/ANK REPEAT), ANKYRIN 2 REPEAT HELIX	COMPLEX (TRANSCRIPTION REG/ANK REPEAT) COMPLEX (TRANSCRIPTION REGULATION/ANK			
	Compound		NF-KAPPA-B P65; CHAIN: A, C; NF-KAPPA-B P50; CHAIN: B, D; I- KAPPA-B-ALPHA; CHAIN: E, F;	NF-KAPPA-B P65; CHAIN: A, C; NF-KAPPA-B P50; CHAIN: B, D; I- KAPPA-B-ALPHA; CHAIN: E, F;	NF-KAPPA-B P65; CHAIN: A, C; NF-KAPPA-B P50; CHAIN: B, D; I- KAPPA-B-ALPHA; CHAIN: E, F;	NF-KAPPA-B P65; CHAIN: A, C; NF-KAPPA-B P50; CHAIN: B, D; I- KAPPA-B-ALPHA; CHAIN: E, F;	NF-KAPPA-B P65; CHAIN: A, C; NF-KAPPA-B P50; CHAIN: B, D; I- KAPPA-B-ALPHA; CHAIN: E, F;
Table 5	SEQ FOLD			94.63			
Tal	PMF		1.00		1.00	1.00	1.00
	Verify score		89.0		0.88	0.77	0.80
	Psi Blast		5.1e-33	1.1e-47	1.2e-46	3.4e-42	1.1e-47
	END		300	241	231	230	203
	START AA		142	42	43	44	6
	CHAIN		ш	ш	ш	E	ш
	PDB ID		1nfi	lnfi	1nfi	1nfi	1nfi
	SEQ ES	E	1430	1430	1430	1430	1430

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	PDB annotation	REPEAT), ANKYRIN 2 REPEAT HELIX	TRANSCRIPTION	REGULATION TRANSCRIPTION	REGULATION, ANKYRIN	REPEATS, CELL-CYCLE	COMPLEX (ANTI- ONCOGENE/ANKYRIN	REPEATS) P53BP2; ANKYRIN	REPEATS, SH3, P53, TUMOK SUPPRESSOR, MULTIGENE 2	FAMILY, NUCLEAR	PROTEIN,	PHOSPHORY LATION, 3 DISEASE MUTATION, 3	POLYMORPHISM, COMPLEX	(ANTI-	ONCOGENE/ANKYRIN	COMPLEX	(INHIBITOR/NUCLEASE)	(INHIBITOR/NUCLEASE),	COMPLEX (RI-ANG),	HYDROLASE 2 MOLECULAR	RECOGNITION, EPITOPE	MAPPING, LEUCINE-RICH 3	COMPLEX (NUCLEAR	
	Compound		REGULATORY PROTEIN SWI6;	CHAIN: A, B;			P53; CHAIN: A; 53BP2; CHAIN: B;									RIBONUCLEASE INHIBITOR;	CHAIN: A, D; ANGIOGENIN;	CHAIN: B, E; 					112 RNA HAIRPIN IV: CHAIN: O.	
Table 5	SEQ FOLD	SCOLE	66.83				66.42																	
Tat	PMF score															0.95							Ç	>>>
	Verify score															0.39	!						0.30	70.0
	Psi Blast		3.4e-18				3.4e-23									3.4e-51	1 1 1						40.05	40-00
	END		285				235									410) •						707	120
	START AA		35				47									153)						700	077
	CHAIN		A				В									4	11							А
	PDB ID		1sw6				1ycs			*			-			19/11	1419						,	layn
	SEQ	NO:	1430) }	•		1430									1/133	CCHI						9	1455

	PDB annotation	PROTEIN/RNA) COMPLEX (NUCLEAR PROTEIN/RNA), PNA	SNRNP, RIBONUCLEOPROTE IN	COMPLEX (NUCLEAR PROTEIN/RNA) COMPLEX (NUCLEAR PROTEIN/RNA).	RNA, SNRNP,RIBONUCLEOPROTE IN	CONTRACTILE PROTEIN LEUCINE-RICH REPEAT,	BETA-BETA-ALPHA	CYLINDEK, DYNEIN, 2 CHLAMYDOMONAS.	FLAGELLA	LIGASE CYCLIN A/CDK2- ASSOCIATED PROTEIN P45;	CYCLIN A/CDK2-	ASSOCIATED PROTEIN P19; SKP1, SKP2, F-BOX, LRR,	LEUCINE-RICH REPEAT,	SCF, UBIQUITIN, 2 E3,	UBIQUITIN FROTEIN LIGASE	LIGASE CYCLIN A/CDK2- ASSOCIATED PROTEIN P45;	CYCLIN A/CDK2-	SKP1, SKP2, F-BOX, LRR,
	Compound	R; U2 A'; CHAIN: A, C; U2 B"; CHAIN: B, D;		U2 RNA HAIRPIN IV; CHAIN: Q, R; U2 A'; CHAIN: A, C; U2 B"; CHAIN: B. D.		OUTER ARM DYNEIN; CHAIN: A;				SKP2; CHAIN: A, C, E, G, I, K, M, O; SKP1; CHAIN: B, D, F, H, J, L,	N, P;					SKP2; CHAIN: A, C, E, G, I, K, M, O; SKP1; CHAIN: B, D, F, H, J, L,	N, P;	
Table 5	SEQ FOLD	SCOR																
Tat	PMF			0.21		0.05				0.70						0.53		
	Verify score			0.29		-0.32				0.29						0.19		
	Psi Blast			1.8e-05		0.0000				8e-12						8.5e-11		
	END AA			375		345				405						400		
	START AA			223		224				196						217		
	CHAIN			O O		А				A						A		,
	PDB ID			1a9n		1ds9				1fqv						1fqv		
	SEQ EQ	 OZ		1433		1433				1433		-				1433		

	uoi	PEAT, E3, IN	CDK2- CYCLIN TED P19; TERRS, PEATS, E3, IN	NAIP; - TEIN FOR IVATING IAIP, UCINE-2 OTEIN, TEIDRAL OHEDRAL	ENAIP; TEIN FOR TVATING VAIP, UCINE- 2 OTEIN, HEDRAL
	PDB annotation	LEUCINE-RICH REPEAT, SCF, UBIQUITIN, 2 E3, UBIQUITIN PROTEIN LIGASE	LIGASE CYCLIN A/CDK2- ASSOCIATED P45; CYCLIN A/CDK2-ASSOCIATED P19; SKP1, SKP2, F-BOX, LRRS, LEUCINE-RICH REPEATS, SCF, 2 UBIQUITIN, E3, UBIQUITIN PROTEIN LIGASE	TRANSCRIPTION RNAIP; RANGAP; GTPASE- ACTIVATING PROTEIN FOR SPI1, GTPASE-ACTIVATING PROTEIN, GAP, RNAIP, RANGAP, LRR, LEUCINE-2 RICH REPEAT PROTEIN, TWINNING, HEMIHEDRAL TWINNING, 3 MEROHEDRAL TWINNING, MEROHEDRAL	TRANSCRIPTION RNAIP; RANGAP; GTPASE- ACTIVATING PROTEIN FOR SPI1, GTPASE-ACTIVATING PROTEIN, GAP, RNAIP, RANGAP, LRR, LEUCINE- 2 RICH REPEAT PROTEIN, TWINNING, 3 MEROHEDRAL TWINNING, 3 MEROHEDRAL
	Compound		SKP2; CHAIN: A, C; SKP1; CHAIN: B, D;	GTPASE-ACTIVATING PROTEIN RNA1_SCHPO; CHAIN: A, B;	GTPASE-ACTIVATING PROTEIN RNA1_SCHPO; CHAIN: A, B;
Table 5	SEQ FOLD				
Tal	PMF		89:0	0.76	0.42
	Verify score		-0.01	0.54	0.48
	Psi Blast		1.7e-11	2e-16	5.1e-07
	END		400	407	409
	START AA		215	194	197
	CHAIN		A	⋖	A
	PDB ID		162	1yrg	1угв
	SEQ ID		1433	1433	1433

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	PDB annotation	TWINNING, MEROHEDRY	TRANSCRIPTION RNA1P; RANGAP; GTPASE- ACTIVATING PROTEIN FOR SPI1, GTPASE-ACTIVATING	PROTEIN, GAP, RNAIP, RANGAP, LRR, LEUCINE- 2 RICH REPEAT PROTEIN, TWINNING, HEMIHEDRAL TWINNING, 3 MEROHEDRAL TWINNING, MEROHEDRY	ACETYLATION RNASE INHIBITOR, RIBONUCLEASE/ANGIOGEN IN INHIBITOR ACETYLATION, LEUCINE- RICH REPEATS		COMPLEX (NUCLEAR PROTEIN/RNA) COMPLEX (NUCLEAR PROTEIN/RNA), RNA,	SNRNP,RIBONUCLEOPROTE IN	RNA BINDING PROTEIN/RNA NESTED DOUBLE PSEUDOKNOT RNA STRUCTURE	RIBONUCLEOPROTEIN U1A117; RIBONUCLEOPROTEIN, RNP
	Compound		GTPASE-ACTIVATING PROTEIN RNA1_SCHPO; CHAIN: A, B;		RIBONUCLEASE INHIBITOR; CHAIN: NULL;		U2 RNA HAIRPIN IV; CHAIN: Q, R; U2 A'; CHAIN: A, C; U2 B"; CHAIN: B, D;		UIA PROTEIN; CHAIN: A; HDV RIBOZYME SELF-CLEAVED; CHAIN: B;	UI SMALL NUCLEAR RIBONUCLEOPROTEIN A; CHAIN: NULL;
Table 5	SEQ FOLD	2006								
Tab	PMF		0.88		0.95	,	0.99		1.00	1.00
	Verify score		0.69		0.47		0.41		0.50	0.48
	Psi Blast		1.2e-08		5.1e-60		3.6e-05		0.00024	3.6e-05
	END		374		410		79		79	79
	START AA		217		153		13		13	13
	CHAIN		А				8		A	
	PDB ID		lyrg		2bnh		1a9n		1cx0	1fht
	SEQ D	 OZ	1433		1433		1440		1440	1440

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	PDB annotation	DOMAIN, SPLICEOSOME	NUCLEAR PROTEIN HETEROGENEOUS	NUCLEAR RIBONUCLEOPROTEIN A1, NUCLEAR PROTEIN, HNRNP,	RBD, RRM, RNP, RNA BINDING, 2 RIBONUCLEOPROTEIN									COMPLEX	(RIBONUCLEOPROTEIN/RNA			NUCLEAR PROTEIN UI
	Compound		HNRNP A1; CHAIN: NULL;			RIBONUCLEOPROTEIN PROTEIN FROM U1 SMALL NUCLEAR	CID INRC 3 (N-TERMINAL FRAGMENT RESIDIFES 1 - 95)	MUTANT WITH GLN 85 INRC 4 REPLACED BY CYS (Q85C) INRC	5	RIBONUCLEOPROTEIN PROTEIN FROM UI SMALL NUCLEAR	KIBONUCLEOPROTEIIN (SINKAF UI) INRC 3 (N-TERMINAL	FRAGMENT, RESIDUES 1 - 95)	REPLACED BY CYS (Q85C) INRC	5 THA SPLICEOSOMAL PROTEIN:	1URN 5 CHAIN: A, B, C; 1URN 6	RNA 21MER HAIRPIN (5'-	(AP*AP*UP*CP*CP*AP*UP*UP* 1URN 11 CHAIN: P, Q, R 1URN 13	UI SMALL NUCLEAR
Table 5	SEQ FOLD	acore																
Tat	PMF score		0.64			0.77				0.58				0.08	?		-	0.04
	Verify score		0.78			-0.21				-0.06				0.77	70			0.34
	Psi Blast		0.0011			0.00012				8.4e-05				VC000 0	1,000.0			0.00012
	END		84			79				78				0,5	6/			82
	START AA		13			13			-	13				12	CI .		,	6
	CHAIN					A				В					∢			
	PDB ID		1ha1			1mc				1nrc					Elmi			2u1a
	SEQ ID	.ON	1440			1440				1440				,	1440			1440

Table 5	

	PDB annotation	SNRNP A PROTEIN; RNA BINDING DOMAIN, NUCLEAR PROTEIN	COMPLEX (RIBONUCLEOPROTEIN/DN A) HNRNP A1, UP1; COMPLEX (RIBONUCLEOPROTEIN/DN A), HETEROGENEOUS NUCLEAR 2 RIBONUCLEOPROTEIN A1	COMPLEX (ZINC FINGER/DNA) COMPLEX (ZINC FINGER/DNA), ZINC FINGER, DNA-BINDING PROTEIN	COMPLEX (ZINC FINGER/DNA) COMPLEX (ZINC FINGER/DNA), ZINC FINGER, DNA-BINDING PROTEIN	COMPLEX (ZINC FINGER/DNA) COMPLEX (ZINC FINGER/DNA), ZINC FINGER, DNA-BINDING PROTEIN	COMPLEX (ZINC FINGER/DNA) COMPLEX (ZINC FINGER/DNA), ZINC FINGER, DNA-BINDING
	Compound	RIBONUCLEOPROTEIN A; CHAIN: NULL;	HETEROGENEOUS NUCLEAR RIBONUCLEOPROTEIN A1; CHAIN: A; 12-NUCLEOTIDE SINGLE-STRANDED TELOMETRIC DNA; CHAIN: B;	QGSR ZINC FINGER PEPTIDE; CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE; CHAIN: B, C;	QGSR ZINC FINGER PEPTIDE; CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE; CHAIN: B, C;	QGSR ZINC FINGER PEPTIDE; CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE; CHAIN: B, C;	QGSR ZINC FINGER PEPTIDE; CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE; CHAIN: B, C;
Table 5	SEQ FOLD score						
Tab	PMF		0.49	0.72	86.0	1.00	1.00
	Verify score		0.43	0.14	0.02	0.31	0.13
	Psi Blast		0.0024	8.8e-29	8.8e-44	8.5e-31	6.6e-44
	END		84	78	215	382	383
	START AA		14	10	134	302	302
	CHAIN		A	A	∀	A	A
	PDB		2up1	1a1h	lalh	lalh	lalh
	SEQ ID		1440	1446	1446	1446	1446

	PDB annotatic
	Compound
ole 5	SEQ
Tal	PMF
	Verify
	Psi
	END
	CHAIN START
	CHAIN

	PDB annotation		PROTEIN	COMPLEX (ZINC FINGER/DNA) COMPLEX	(ZINC FINGER/DNA), ZINC	FINGER, DNA-BINDING PROTEIN	COMPLEX (ZINC	(ZINC FINGER/DNA), ZINC	FINGER, DNA-BINDÍNG PROTEIN	COMPLEX (ZINC	FINGER/DNA) COMPLEX	(ZINC FINGER/DNA), ZINC	FINGER, DNA-BINDING	PROTEIN	COMPLEX (ZINC FINGER, FINGER,	PROTEIN-DNA	INTERACTION, PROTEIN	DESIGN, 2 CRYSTAL	STRUCTURE, COMPLEX	(ZINC FINGER/DNA)	COMPLEX (ZINC	FINGER/DNA) ZINC FINGER,	PROTEIN-DNA	INTERACTION, PROTEIN	DESIGN, 2 CRYSTAL	STRUCTURE, COMPLEX	(ZINC FINGER/DINA)	COMPLEX (ZINC
	Compound			QGSR ZINC FINGER PEPTIDE; CHAIN: A: DUPLEX	OLIGONUCLEOTIDE BINDING	SITE; CHAIN: B, C;	QGSR ZINC FINGER PEPTIDE;	CHAIN: A; DOFLEA OI IGONI ICI FOTTDE BINDING	SITE; CHAIN: B, C;	QGSR ZINC FINGER PEPTIDE;	CHAIN: A; DUPLEX	OLIGONUCLEOTIDE BINDING	SITE; CHAIN: B, C;		DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER	PROTEIN; CHAIN: C, F, G;					DNA; CHAIN: A, B, D, E;	CONSENSUS ZINC FINGER	PROTEIN; CHAIN: C, F, G;					DNA; CHAIN: A, B, D, E;
Table 5	SEQ	FOLD		80.03					,																			
Tak	PMF	score					0.71			0.48					0.93						1.00							1.00
:	Verify	score					-0.28			-0.01					-0.08						0.33							0.42
	Psi	Blast		6.6e-44			5.1e-26			4.4e-36					3.4e-43						1.2e-47							1.5e-49
	END	AA		412			77	-		187		***			186						214							242
	START	AA		330			4			81	()				109						133	1						161
	CHAIN	А		A			A			A	4				S						C)						၁
	PDB	<u> </u>		lalh	_		lalh			1a1h					1mey						1mev	Commit						1mey
	SEQ	A Š		1446			1446			1446	2				1446						1446	2						1446

	PDB annotation	FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN	DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA)	COMPLEX (ZINC FINGER/DNA) ZINC FINGER,	PROTEIN-DNA INTERACTION, PROTEIN	DESIGN, 2 CRYSTAL	STRUCTURE, COMPLEX (ZINC FINGER/DNA)	COMPLEX (ZINC FINGER/DNA) ZINC FINGER.	PROTEIN-DNA	INTERACTION, PROTEIN	DESIGN, 2 CRYSTAL	STRUCTURE, COMPLEX	(ZINC FINGER/DINA)	COMPLEX (ZINC FINGER/DNA) ZINC FINGER,	PROTEIN-DNA	INTERACTION, PROTEIN	DESIGN, 2 CRYSTAL	STRUCTURE, COMPLEX	(ZINC FINGER/DNA)	COMPLEX (ZINC	FINGER/DINA) ZINC FINGER, DROTEIN-DINA	INTERACTION, PROTEIN
	Compound	CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G;		DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER	PROTEIN; CHAIN: C, F, G;			DNA; CHAIN: A, B, D, E;	PROTEIN; CHAIN: C, F, G;				5 6	DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER	PROTEIN; CHAIN: C, F, G;					DNA; CHAIN: A, B, D, E;	CONSENSUS ZINC FINGER	rrolem, Cham. C, r, G,
Table 5	SEQ FOLD score							100.67														
Tat	PMF			1.00										1.00						1.00		
	Verify score			0.45										0.45						0.38		
	Psi Blast			5.1e-50				8.5e-51						8.5e-51						5.1e-45		
	END			270				271	-					298						105		
	START AA			189				189						217						24		
	CHAIN			၁				C						ပ						S		
	PDB ID			lmey				1mey						1mey						lmey		
	SEQ Signal Seq			1446				1446						1446						1446		

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	PDB annotation	DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA)	COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL	SIRUCIURE, COMPLEX (ZINC FINGER/DNA)	COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN, DNA	INTERACTION, PROTEIN DESIGN, 2 CRYSTAL	STRUCTURE, COMPLEX (ZINC FINGER/DNA)	COMPLEX (ZINC FINGER,	PROTEIN-DNA	INTERACTION, PROTEIN DESIGN, 2 CRYSTAL	STRUCTURE, COMPLEX (ZINC FINGER/DNA)	COMPLEX (ZINC FINGER FINGER	PROTEIN-DNA	INTERACTION, PROTEIN	DESIGN, 2 CRYSTAL	(ZINC FINGER/DNA)
	Compound		DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G;		DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER	FROIEIN, CIPAIN. C, 1, C,		DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER	PROTEIN; CHAIN: C, F, G;			DNA; CHAIN: A, B, D, E;	PROTEIN; CHAIN: C, F, G;			
Table 5	SEQ FOLD score															
Tab	PMF		1.00		1.00			1.00				1.00				
	Verify score		0.34		60.0			0.14				-0.02				
	Psi Blast		3.4e-50		6.8e-50			8.5e-40				5.1e-50				
	END AA		326		354			77				382				
	START AA		245		273			3				301				
	CHAIN		S		ပ			C				ပ				
	PDB		1mey	•	1mey	1		Imey				1mey				
	SEQ D	Cu	1446		1446			1446				1446				

	PDB annotation	COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA	INTERACTION, PROTEIN	DESIGN, 2 CRYSTAL	STRUCTURE, COMPLEX (ZINC FINGER/DNA)	COMPLEX (ZINC FINGER/DNA) ZINC FINGER,	PROTEIN-DNA	INTERACTION, PROTEIN	DESIGN, 2 CRYSTAL	STRUCTURE, COMPLEX	(ZINC FINGER/DNA)	COMPLEX (ZINC FINGER,	PROTEIN-DNA	INTERACTION, PROTEIN	DESIGN, 2 CRYSTAL	STRUCTURE, COMPLEX	(ZINC FINGER/DNA)	COMPLEX (ZINC	FINGER/DNA) ZINC FINGER,	PROTEIN-DNA	INTERACTION, PROTEIN	DESIGN, 2 CRYSTAL	STRUCTURE, COMPLEX	(ZINC FINGER/DNA)	COMPLEX (TRANSCRIPTION	REGULATION/DNA) COMPLEX (TRANSCRIPTION
	Compound	DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN: CHAIN: C. F. G.				DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER	PROTEIN; CHAIN: C, F, G;					DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER	PROTEIN; CHAIN: C, F, G;					DNA; CHAIN: A, B, D, E;	CONSENSUS ZINC FINGER	PROTEIN; CHAIN: C, F, G;					TFIIIA; CHAIN: A, D; 5S	RIBOSOMAL RNA GENE; CHAÎN: B, C, E, F;
Table 5	SEQ FOLD score																									
Tak	PMF	1.00				1.00						0.82						0.98					-		69.0	
	Verify score	0.19				0.18						-0.26						0.37							-0.40	
	Psi Blast	3.4e-50		•		6.8e-42						2.2e-37						5.1e-11							1.1e-56	,
	END	410			-	130				·		186						49							214	
	START AA	329				52						81						22	1						10	
	CHAIN ID	O				C						၁						٢)						A	
	PDB ID	1mey				1mey						1mey						1mev	- Carrie						1tf6	
	SEQ S D SEQ					1446						1446						1446	2						1446	:

Γ		T			7 7	7.
	PDB annotation	REGULATION/DNA), RNA POLYMERASE III, 2 TRANSCRIPTION INITIATION, ZINC FINGER PROTEIN	COMPLEX (TRANSCRIPTION REGULATION/DNA) COMPLEX (TRANSCRIPTION REGULATION/DNA), RNA POLYMERASE III, 2 TRANSCRIPTION INITIATION, ZINC FINGER PROTEIN	COMPLEX (TRANSCRIPTION REGULATION/DNA) COMPLEX (TRANSCRIPTION REGULATION/DNA), RNA POLYMERASE III, 2 TRANSCRIPTION INITIATION, ZINC FINGER PROTEIN	COMPLEX (TRANSCRIPTION REGULATION/DNA) COMPLEX (TRANSCRIPTION REGULATION/DNA), RNA POLYMERASE III, 2 TRANSCRIPTION INITIATION, ZINC FINGER PROTEIN	COMPLEX (TRANSCRIPTION REGULATION/DNA)
	Compound		TFIIIA; CHAIN: A, D; 5S RIBOSOMAL RNA GENE; CHAIN: B, C, E, F;	TFIIIA; CHAIN: A, D; 5S RIBOSOMAL RNA GENE; CHAIN: B, C, E, F;	TFIIIA; CHAIN: A, D; 5S RIBOSOMAL RNA GENE; CHAIN: B, C, E, F;	TFIIIA; CHAIN: A, D; 5S RIBOSOMAL RNA GENE; CHAIN:
Table 5	SEQ FOLD			112.82		
Tac	PMF		0.98		0.72	0.70
	Verify score		-0.07		-0.10	-0.34
	Psi Blast		8.5e-35	6.6e-72	6.6e-72	2.2e-75
	END		251	299	326	410
	START AA		113	133	134	218
	CHAIN		∢	∢	A	A
	PDB ID		1116	1116	14f6	1tf6
	SEQ B	ÖZ	1446	1446	1446	1446

	PDB annotation		COMPLEX (TRANSCRIPTION REGULATION/DNA), RNA POLYMERASE III, 2	TRANSCRIPTION INITIATION, ZINC FINGER	PROTEIN	COMPLEX (TRANSCRIPTION REGULATION/DNA)	COMPLEX (TRANSCRIPTION PEGIT ATTON/DNA) RNA	POLYMERASE III, 2	I KANSCKLFI I ON INITIATION ZINCEINGER	PROTEIN	COMPLEX (TRANSCRIPTION	REGULATION/DNA)	COMPLEX (TRANSCRIPTION DECIM ATTON/ONA) RNA	POI VMER ASE III 2	TEANSCRIPTION	INITIATION, ZINC FINGER	PROTEIN	COMPLEX (TRANSCRIPTION	REGULATION/DNA)	COMPLEX (TRANSCRIPTION	REGULATION/DNA), RNA	POLYMERASE III, 2	TRANSCRIPTION	INITIATION, ZINC FINGER	PROTEIN CONTRIET THE ANSCRIPTION	COMPLEA (IRAINSCRIFIIOIN
	Compound		B, C, E, F;			TFIIIA; CHAIN: A, D; 5S RIBOSOMAL RNA GENE; CHAIN:	B, C, E, F;				TFIIIA; CHAIN: A, D; 5S	RIBOSOMAL RNA GENE; CHAIN:	B, C, E, F;					TFIIIA; CHAIN: A, D; 5S	RIBOSOMAL RNA GENE; CHAIN:	B, C, E, F;					Ch H i I'll and i manner	THIIIA; CHAIN: A, D; 58
Table 5	SEQ	FOLD																								
Taf	PMF	score				86.0					1.00							0.98								1.00
	Verify	score				-0.29					0.01							-0.21								-0.08
	Psi	Blast		,,		1.7e-38					8.5e-36							8.5e-33								2.2e-71
	END	AA				392					410							144								270
	START	AA				246					274							3	1							81
	CHAIN					A					4	.						A	17							А
	PDB	<u></u>			-	1tf6					1+fk	2						1+fK	211							1tf6
	SEQ	n e				1446			•		1446	2						1446	7							1446

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	PDB annotation	REGULATION/DNA) COMPLEX (TRANSCRIPTION REGULATION/DNA), RNA POLYMERASE III, 2	TRANSCRIPTION INITIATION, ZINC FINGER PROTEIN	COMPLEX (TRANSCRIPTION REGULATION/DNA) YING-	YANG 1; TRANSCRIPTION INITIATION, INITIATOR	ELEMENT, YY1, ZINC 2	PROTEIN RECOGNITION, 3	COMPLEX (TRANSCRIPTION	REGULATION/DINA)	COMPLEX (TRANSCRIPTION PECITY ATTOMONA) VING	YANG 1; TRANSCRIPTION	INITIATION, INITIATOR	ELEMENT, YY1, ZINC 2	PROTEIN RECOGNITION 3	COMPLEX (TRANSCRIPTION	REGULATION/DNA)	COMPLEX (TRANSCRIPTION	REGULATION/DNA) YING- YANG 1: TRANSCRIPTION	INITIATION, INITIATOR	ELEMENT, YY1, ZINC 2 FINGER PROTEIN, DNA-
	Compound	RIBOSOMAL RNA GENE; CHAIN: B, C, E, F;		YY1; CHAIN: C; ADENO- ASSOCIATED VIRUS P5	INITIATOR ELEMENT DNA; CHAIN: A, B;					YY1; CHAIN: C; ADENO-	ASSOCIATED VIRUS F3 INITIATOR ELEMENT DNA;	CHAIN: A, B;					YY1; CHAIN: C; ADENO-	ASSOCIATED VIRUS P5 INITIATOR FLEMENT DNA:	CHAIN: A, B;	
Table 5	SEQ FOLD score																69.68		<u> </u>	
Tat	PMF			1.00						0.95										
	Verify score			0.16						-0.07										
	Psi Blast			6.6e-38						8.8e-48							1.5e-57			
	END			105						242							243			
	START			10						106							133			
	CHAIN			S						C		-					O			
	PDB ID			1ubd						1ubd							lubd			
	SEQ ID			1446						1446							1446			

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	PDB annotation		PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULATION/DNA)	COMPLEX (TRANSCRIPTION	REGULATION/DNA) YING- YANG 1; TRANSCRIPTION	INITIATION, INITIATOR	ELEMENT, YY1, ZINC 2	FINGER PROTEIN, DNA-	PROTEIN RECOGNITION, 3	COMPLEX (TRANSCRIPTION	KEGOLATION/DIVA)	COMPLEX (TRANSCRIPTION	KEGULA IION/DNA) YING-	YANG I; TRANSCRIPTION	INITIATION, INITIATOR	ELEMENT, YY1, ZINC 2	FINGER PROTEIN, DNA-	PROTEIN RECOGNITION, 3	COMPLEX (TRANSCRIPTION	REGULATION/DNA)	COMPLEX (TRANSCRIPTION	REGULATION/DNA) YING-	YANG 1; TRANSCRIPTION	INITIATION, INITIATOR	ELEMENT, YY1, ZINC 2	FINGER PROTEIN, DNA-	PROTEIN RECOGNITION, 3	COMPLEX (TRANSCRIPTION	REGULATION/DNA)	COMPLEX (TRANSCRIPTION
	Compound			YY1; CHAIN: C; ADENO-	ASSOCIATED VIRUS P5" INITIATOR ELEMENT DNA:	CHAIN: A, B;						YY1; CHAIN: C; ADENO-	ASSOCIATED VIRUS PS	INITIATOR ELEMENT DNA;	CHAIN: A, B;						YY1; CHAIN: C; ADENO-	ASSOCIATED VIRUS P5	INITIATOR ELEMENT DNA;	CHAIN: A, B;						YY1; CHAIN: C; ADENO-
Table 5	SEQ	FOLD								,																				
Tal	PMF	score		1.00								0.98									0.34									1.00
	Verify	score		0.29								-0.07									0.05									-0.08
	Psi	Blast		1.5e-57								6.6e-54									1.8e-52									3.4e-36
	END	AA		270								326									382									382
	START	AA		159								215									243		_							278
	CHAIN	A		C	,							O			_						S									၁
	PDB	<u></u>		1ubd								1ubd			•	•					1ubd						_			1ubd
	SEQ	—— 日 🞖		1446								1446									1446									1446

	PDB annotation	REGULATION/DNA) YING- YANG 1; TRANSCRIPTION INITIATION, INITIATOR ELEMENT, YY1, ZINC 2 FINGER PROTEIN, DNA- PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRIPTION	REGULATION/DNA) COMPLEX (TRANSCRIPTION REGULATION/DNA) YING- VANG 1: TRANSCRIPTION	INITIATION, INITIATOR ELEMENT, YY1, ZINC 2 FINGER PROTEIN, DNA-	PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULATION/DNA)	COMPLEX (TRANSCRIPTION REGULATION/DNA) YING-YANG 1: TRANSCRIPTION	INTTIATION, INITIATOR ELEMENT, YY1, ZINC 2 FINGER PROTEIN, DNA- PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULATION/DNA)	COMPLEX (TRANSCRIPTION REGULATION/DNA) YING- YANG 1; TRANSCRIPTION INITIATION, INITIATOR ELEMENT, YY1, ZINC 2
	Compound	ASSOCIATED VIRUS P5 INITIATOR ELEMENT DNA; CHAIN: A, B;	YY1; CHAIN: C; ADENO- ASSOCIATED VIRUS P5	CHAIN: A, B;		YY1; CHAIN: C; ADENO- ASSOCIATED VIRUS P5 NITIATOR ELEMENT DNA:	CHAIN: A, B;	YYI; CHAIN: C; ADENO- ASSOCIATED VIRUS P5 INITIATOR ELEMENT DNA; CHAIN: A, B;
Table 5	SEQ FOLD score							
Tat	PMF		1.00			0.90		86.0
	Verify score		0.18			0.17		-0.05
	Psi Blast		6.6e-56			1.2e-34		1.7e-30
	END AA		410			410		130
	START AA		299			309		32
	CHAIN ID		O O			O		O O
	PDB ID		1ubd			1ubd		lubd
	SEQ EQ		1446			1446	-	1446

																						_							
	PDB annotation		FINGER PROTEIN, DNA- PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRIPTION	REGULATION/DNA)	COMPLEX (TRANSCRIPTION REGULATION/DNA) YING-	YANG 1; TRANSCRIPTION	INITIATION, INITIATOR ELEMENT, YY1, ZINC 2	FINGER PROTEIN, DNA-	PROTEIN RECOGNITION, 3	COMPLEX (TRANSCRIPTION	REGULATION/DNA)	COMPLEX (TRANSCRIPTION	REGULATION/DNA) YING-	YANG 1; TRANSCRIPTION	INITIATION, INITIATOR	ELEMENT, YY1, ZINC 2	FINGER PROTEIN, DNA-	PROTEIN RECOGNITION, 3	COMPLEX (TRANSCRIPTION	REGULATION/DNA)	COMPLEX (DNA-BINDING	PROTEIN/DNA) FIVE-	FINGER GLI; GLI, ZINC	FINGER, COMPLEX (DNA-	BINDING PROTEIN/DNA)	COMPLEX (DNA-BINDING	PROTEIN/DNA) FIVE-	FINGER GLI; GLI, ZINC	FINGER, COMPLEX (DNA-
	Compound				YY1; CHAIN: C; ADENO- ASSOCIATED VIRUS P5	INITIATOR ELEMENT DNA;	CHAIN: A, B;					YY1; CHAIN: C; ADENO-	ASSOCIATED VIRUS P5	INITIATOR ELEMENT DNA;	CHAIN: A, B;						ZINC FINGER PROTEIN GLI1;	CHAIN: A; DNA; CHAIN: C, D;				ZINC FINGER PROTEIN GLI1;	CHAIN: A; DNA; CHAIN: C, D;		
Table 5	SEQ FOLD	score					1																			101.80			
Tal	PMF score				1.00							0.99									0.99								
	Verify score				0.19							-0.09									-0.09								
	Psi Blast				3.4e-31							2.2e-45									1e-33	1		•		1.1e-71			
	END				105							186									241	: 1				272	 - 		
	START				4		_					50	,	,							113	}				133	1		
	CHAIN	***			C							C	- 								4	17				4	4		
	PDB ID				lubd							luhd	201								Jali	7 E E II				2oli	7,811		
	SEQ	ÖN			1446							1446	2								1446	044				1446	<u> </u>		

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	PDB annotation		BINDING PROTEIN/DNA)	COMPLEX (DNA-BINDING PROTEINDINA) FIVE.	FINGER GLI, GLI, ZINC	FINGER, COMPLEX (DNA-	BINDING PROTEIN/DNA)	COMPLEX (DNA-BINDING	PROTEIN/DNA) FIVE-	FINGER, CLI, CLI, CHAC	BINDING PROTEIN/DNA)	COMPLEX (DNA-BINDING	PROTEIN/DNA) FIVE-	FINGER GLI; GLI, ZINC	FINGER, COMPLEX (DNA-	BINDING PROTEIN/DNA)	COMPLEX (DNA-BINDING	PROTEIN/DNA) FIVE-	FINGER GLI; GLI, ZINC	FINGER, COMPLEX (DNA-	BINDING PROTEIN/DNA)	COMPLEX (DNA-BINDING	PROTEIN/DNA) FIVE-	FINGER GLI; GLI, ZINC	FINGER, COMPLEX (DNA-	BINDING PROTEIN/DNA)	COMPLEX (DNA-BINDING	PROTEIN/DNA) FIVE-	FINGER GLI; GLI, ZINC	FINGER, COMPLEX (DNA-	BINDING PROTEIN/DNA)
	Compound		-	ZINC FINGER PROTEIN GLI1;	CHAIN: A, DINA, CHAIN: C, L,	,		ZINC FINGER PROTEIN GLI1;	CHAIN: A; DNA; CHAIN: C, D;			ZINC FINGER PROTEIN GLII;	CHAIN: A; DNA; CHAIN: C, D;				ZINC FINGER PROTEIN GLI1;	CHAIN: A; DNA; CHAIN: C, D;				ZINC FINGER PROTEIN GLI1;	CHAIN: A; DNA; CHAIN: C, D;				ZINC FINGER PROTEIN GLI1;	CHAIN: A; DNA; CHAIN: C, D;			
Table 5	SEQ	FOLD																													
Tal	PMF	score		1.00				0.88				0.99					1.00					1.00					1.00				
	Verify	score		0.61				0.03				0.08					0.12					0.23					0.15				
	Psi	Blast		1.1e-71		.,, .		8.8e-70				8.8e-58					1.3e-72					1.7e-34					1.2e-34)) !			
	END	AA		272				356				188)				411					381					409	<u>}</u>			
	START	AA		134				190				24					245					253					281	107			
	CHAIN	А		A				A				٨	.				⋖	•				4	1				V	17			
	PDB	A		2gli				2gli		-		20li	7				20li	ņ				2oli	i i				20li	7 2 N			
	SEQ	ДŞ		1446				1446				1446	2				1446	2				1446	2				1446	0+4-1			

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	PDB annotation	COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE- FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA)	LIPID TRANSPORT APO A-I; LIPOPROTEIN, LIPID TRANSPORT,	CHOLESTEROL METABOLISM, 2 ATHEROSCLEROSIS, HDL, LCAT-ACTIVATION	ENDOCYTOSIS/EXOCYTOSI S NSEC1; PROTEIN-PROTEIN COMPLEX, MULTI-SUBUNIT	TRANSFERASE ALPHA- SUPERHELIX, TRANSFERASE	CONTRACTILE PROTEIN TRIPLE-HELIX COILED COIL, CONTRACTILE PROTEIN	LIPID TRANSPORT APO A-I; LIPOPROTEIN, LIPID TRANSPORT, CHOLESTEROL METABOLISM, 2 ATHEROSCLEROSIS, HDL, LCAT-ACTIVATION
	Compound	ZINC FINGER PROTEIN GLI1; CHAIN: A; DNA; CHAIN: C, D;	A, B, C, D;		SYNTAXIN BINDING PROTEIN 1; CHAIN: A; SYNTAXIN 1A; CHAIN: B;	SOLUBLE LYTIC TRANSGLYCOSYLASE SLT70; CHAIN: A;	HUMAN SKELETAL MUSCLE ALPHA-ACTININ 2; CHAIN: A;	APOLIPOPROTEIN A-I; CHAIN: A, B, C, D;
Table 5	SEQ FOLD score		60.91					61.06
Tat	PMF	1.00			-0.11	-0.13	-0.18	
	Verify score	0.07			0.16	0.01	0.17	
	Psi Blast	3.4e-30	1.2e-09		3.6e-08	7.2e-12	2.4e-09	1.2e-09
	END AA	132	255		197	313	200	232
	START AA	4	61		85	09	84	15
	CHAIN D	A	A		B	А	A	A
	PDB ID	2gli	lavi		1dn1	Iqsa	1quu	lav1
	SEQ NO B	 	1447		1447	1447	1447	1448

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	PDB annotation		ENDOCYTOSIS/EXOCYTOSI S NSEC1; PROTEIN-PROTEIN COMPLEX, MULTI-SUBUNIT	PROTEIN TRANSPORT HELIX-TURN-HELIX TPR- LIKE REPEAT, PROTEIN TRANSPORT	TRANSFERASE ALPHA- SUPERHELIX, TRANSFERASE	COMPLEX (ZINC	FINGER/DNA) COMPLEX (ZINC FINGER/DNA), ZINC FINGER, DNA-BINDING	PROTEIN	COMPLEX (ZINC FINGER, FINGER, ZINC FINGER,	PROTEIN-DNA INTERACTION, PROTEIN	DESIGN, 2 CRYSTAL	STRUCTURE, COMPLEX (ZINC FINGER/DNA)	COMPLEX (ZINC	FINGER/DNA) ZINC FINGER,	INTERACTION, PROTEIN	DESIGN, 2 CRYSTAL	STRUCTURE, COMPLEX	COMPLEX (ZINC	
	Compound		SYNTAXIN BINDING PROTEIN 1; CHAIN: A; SYNTAXIN 1A; CHAIN: B;	VESICULAR TRANSPORT PROTEIN SEC17; CHAIN: A;	SOLUBLE LYTIC TRANSGLYCOSYLASE SLT70; CHAIN: A;	OGSR ZINC FINGER PEPTIDE:	CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE; CHAIN: B, C;		DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER	PROTEIN; CHAIN: C, F, G;			DNA; CHAIN: A, B, D, E;	CONSENSUS ZINC FINGER	FROIDIN, CHAIN. C, I, C,			DNA; CHAIN: A, B, D, E;	
Table 5	SEQ	FOLD																	
Tat	PMF	score	-0.11	0.07	-0.09	0.73			1.00				1.00					1.00	
	Verify	score	0.16	-0.09	0.10	0.53))		0.31				0.35	:				0.58	
	Psi	Blast	3.6e-08	0.00036	2.4e-12	2 40 72	7.45-6		3.4e-42				8.5e-44					1e-44	
	END	AA	197	318	319	150	oct.		206				234					262	
	START	AA	85	84	09	O.F.	2		125				153			-		181	
	CHAIN	<u> </u>	В	Ą	A		¥		S				C)				O O	,
	PDB	<u>A</u>	1dn1	1qqe	1qsa		lain	-	Imey		-		1 mev	(Sum)				1mev	(2000)
	SEQ	<u>a Ş</u>	1448	1448	1448	,	1451		1451				1451	1				1451	1

	PDB annotation	FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN	DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA)	COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA	INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX	(ZINC FINGER/DNA)	COMPLEX (ZINC FINGER,	PROTEIN-DNA INTERACTION PROTEIN	DESIGN, 2 CRYSTAL	STRUCTURE, COMPLEX	COMPLEY (ZINC	FINGER/DNA) ZINC FINGER,	PROTEIN-DNA	INTERACTION, PROTEIN DESIGN, 2 CRYSTAL	STRUCTURE, COMPLEX	(ZINC FINGER/DNA)	COMPLEX (ZINC FINGER/DNA) ZINC FINGER,	PROTEIN-DNA INTERACTION, PROTEIN
	Compound	CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G;		DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN: CHAIN: C. F. G;			DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER	PROTEIN; CHAIN: C, F, G;			PATA CITABLA D. D.	DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER	PROTEIN; CHAIN: C, F, G;				DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER	PROTEIN; CHAIN: C, F, G;
Table 5	SEQ FOLD score		-															
Tab	PMF score			1.00			1.00				,	00: 1:00					1.00	
	Verify			-0.03			0.15					0.40					0.73	
	Psi Blast			1.2e-45			1.4e-46				!	3.4e-47					1.4e-48	
	END			290			318					346					374	
	START			209			237					265					293	
	CHAIN			2			C					ပ					ပ	
	PDB ID			1mey			1mey					1mey	_		-		lmey	
	SEQ ID			1451			1451	,				1451					1451	

	PDB annotation		DESIGN, 2 CRYSTAL	STRUCTURE, COMPLEX (ZINC FINGER/DNA)	COMPLEX (ZINC	FINGER/DNA) ZINC FINGER,	PROTEIN-DNA	INTERACTION, PROTEIN	DESIGN, 2 CRYSTAL	STRUCTURE, COMPLEX	(ZINC FINGER/DNA)	COMPLEX (ZINC	FINGER/DNA) ZINC FINGER,	PROTEIN-DNA	INTERACTION, PROTEIN	DESIGN, 2 CRYSTAL	STRUCTURE, COMPLEX	(ZINC FINGER/DNA)	COMPLEX (ZINC	FINGER/DNA) ZINC FINGER,	PROTEIN-DNA	INTERACTION, PROTEIN	DESIGN, 2 CRYSTAL	STRUCTURE, COMPLEX	(ZINC FINGER/DNA)	COMPLEX (ZINC	FINGER/DNA) ZINC FINGER,	PKOLEIN-DINA	INTERACTION, PROTEIN	DESIGN, 2 CRYSTAL	STRUCTURE, COMPLEX (ZINC FINGER/DNA)	
	Compound				DNA: CHAIN: A. B. D. E.	CONSENSUS ZINC FINGER	PROTEIN; CHAIN: C, F, G;					DNA; CHAIN: A, B, D, E;	CONSENSUS ZINC FINGER	PROTEIN; CHAIN: C, F, G;					DNA; CHAIN: A, B, D, E;	CONSENSUS ZINC FINGER	PROTEIN; CHAIN: C, F, G;					DNA; CHAIN: A, B, D, E;	CONSENSUS ZINC FINGER	PROTEIN; CHAIN: C, F, G;				
Table 5	SEQ	FOLD																														
Tak	PMF	score			1 00	2						1.00							1.00							1.00						
	Verify	score			0.11	7.7						0.27	į						0.42	!						0.75						
	Psi	Blast			1 70 40	1.1						5 1e-50	2						5 1e-50							1e-50						
	END	AA		1112	400	701					v 	430	2			•			458	5						486						
	START	AA			271	175						340	ì		•				277							405						
	CHAIN	<u></u>)						C)			-		
	PDB				+	ımey						+	ıııey			•			╁	, illey	•					1mev						
	SEQ	G Ş	OZI		+	1451						1451	1451						17451	1471						1451						

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	PDB annotation		COMPLEX (ZINC FINGER, FINGER,	PROTEIN-DNA	INTERACTION, PROTEIN	DESIGN, 2 CRYSTAL	STRUCTURE, COMPLEX	(ZINC FINGER/DNA)	COMPLEX (ZINC	PROTEIN-DNA	INTERACTION, PROTEIN	DESIGN, 2 CRYSTAL	STRUCTURE, COMPLEX	(ZINC FINGER/DNA)	COMPLEX (ZINC	FINGER/DNA) ZINC FINGER,	PROTEIN-DNA	INTERACTION, PROTEIN	DESIGN, 2 CRYSTAL	STRUCTURE, COMPLEX	(ZINC FINGER/DNA)	COMPLEX (ZINC	FINGER/DNA) ZINC FINGER,	PROTEIN-DNA	NTERACTION, PROTEIN	DESIGN, 2 CRYSTAL	STRUCTURE, COMPLEX	(ZINC FINGER/DNA)	COMPLEX (ZINC	PROTEIN-DNA	
	Compound		DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER	PROTEIN; CHAIN: C, F, G;					DNA; CHAIN: A, B, D, E;	CONSENSOS ZINC FINGER PROTEIN: CHAIN: C F G:	INCIERT, CHEMIN CO. 1, C,				DNA; CHAIN: A, B, D, E;	CONSENSUS ZINC FINGER	PROTEIN; CHAIN: C, F, G;					DNA; CHAIN: A, B, D, E;	CONSENSUS ZINC FINGER	PROTEIN; CHAIN: C, F, G;					DNA; CHAIN: A, B, D, E;	PROTEIN; CHAIN: C. F. G:	, , , , , , , , , , , , , , , , , , , ,
Table 5	SEQ FOLD	score													105.19																
Tab	PMF		1.00						1.00													1.00							1.00		
	Verify score		0.53						0.59													0.47							0.25		
	Psi Blast		6.8e-50	•					8.5e-51	***		•			8.5e-51							1.4e-50							1.4e-50		
	END		514						542						543	!						570							865		
	START AA		433						461				-		461							489							517		
	CHAIN		C						C			_			<u>ر</u>)						C)						C		
	PDB U		1mey		-				1mey		•				1 mev	Commit			•	_		1mev							1mey		
	SEQ	Ö	1451						1451						1451	101						1451	1						1451		

	PDB annotation	INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA)	COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA)	COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA)	COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA)	COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX
	Compound	,	DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G;	DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G;	DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G;	DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G;
Table 5	SEQ FOLD score					
Tak	PMF		1.00	0.31	0.92	1.00
	Verify score		0.05	-0.42	-0.37	1.07
	Psi Blast		5.1e-35	3.46-40	3.4e-41	1.2e-13
	END AA		603	150	178	542
	START AA		545	69	26	515
	CHAIN		O	U	O	ڻ ن
	PDB ID		1mey	1mey	1mey	Imey
	SEQ EQ		1451	1451	1451	1451

\$ S.	PDB annotation		(ZINC FINGER/DNA)	COMPLEX (ZINC FINGER, TINGER, DINC FINGER, D	PROTEIN-DNA	INTERACTION, PROTEIN	DESIGN, 2 CRYSTAL	STRUCTURE, COMPLEX (ZINC FINGER/DNA)	COMPLEX (TRANSCRIPTION	REGULATION/DNA)	COMPLEX (TRANSCRIPTION	REGULATION/DNA), RNA	POLYMERASE III, 2	TRANSCRIPTION	INITIATION, ZINC FINGER	PROTEIN	COMPLEX (TRANSCRIPTION	REGULATION/DNA)	COMPLEX (TRANSCRIPTION	REGULATION/DNA), RNA	POLYMERASE III, 2	TRANSCRIPTION	INITIATION, ZINC FINGER	PROTEIN	COMPLEX (TRANSCRIPTION	REGULATION/DNA)	COMPLEX (TRANSCRIPTION	REGULATION/DNA), KNA	POLYMEKASE III, 2	I KANSCKIF I I ON INITIATION, ZINC FINGER
	Compound			DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER	PROTEIN; CHAIN: C, F, G;				TEITIA: CHAIN: A D: 5S	RIBOSOMAL RNA GENE; CHAIN:	B, C, E, F;						TFIIIA; CHAIN: A, D; 5S	RIBOSOMAL RNA GENE; CHAIN:	B, C, E, F;						TFIIIA; CHAIN: A, D; 5S	RIBOSOMAL RNA GENE; CHAIN:	B, C, E, F;			
Table 5	SEQ	FOLD																								-				
Tal	PMF	score		1.00					0.00	7							89.0								0.95					
	Verify	score		1.07					0.00	70:0							-0.13								0.11					
	Psi	Blast		3.4e-13		-			17021	1.75-54							4.8e-60	: :				-			1.7e-36					
	END	AA		542					720	0/7							318	2							331					
	START	AA		515					701	071							126	77							182					
	CHAIN	А		Ð				<u>.</u>		Ą							4	ς.							A					
	PDB	А		1mey	·				25	0111	•						1+fK	011							11466	2				
	SEQ	 음 [']	j S	1451					;	1451			•				1451	17							1451	1				

			NO	NC					Z		Z						Z	z							Z,	;	z		
DDR annotation	L D.D. almiotation	PROTEIN	COMPLEX (TRANSCRIPTION REGULATION/DNA)	COMPLEX (TRANSCRIPTION	REGULATION/DNA), RNA	FOL YMEKASE III, 2	TRANSCRIPTION DITTION TRICED	INTITATION, CINC FINGER PROTEIN	COMPLEX (TRANSCRIPTION	REGULATION/DNA)	COMPLEX (TRANSCRIPTION	REGULATION/DNA), RNA	POLYMERASE III, 2	TRANSCRIPTION	INITIATION, ZINC FINGER	PROTEIN	COMPLEX (TRANSCRIPTION REGIT ATTOM/DNA)	COMPLEX (TRANSCRIPTION	REGIII ATION/DNA) RNA	DOI VALED A SE III 2	TO LIMITABLE IN, Z	I NAINSCAIL I IOIN	INITIATION, ZINC FINGER	PKO1EIN	COMPLEX (TRANSCRIPTION	KEGULA HON/DINA)	COMPLEX (TRANSCRIPTION	REGULATION/DNA), RNA	POLYMERASE III, 2 TRANSCRIPTION
Commonne	Oumoding		TFIIIA; CHAIN: A, D; 5S RIBOSOMAL RNA GENE; CHAIN:	B, C, E, F;					TFIIIA; CHAIN: A, D; 5S	RIBOSOMAL RNA GENE; CHAIN:	B, C, E, F;				•		TFIIIA; CHAIN: A, D; 5S RIBOSOMAI RNA GENF: CHAIN:	B C F F.	, (, (, (, (, (, (, (, (, (, (, (, (, (,					\$ 1 manual manua	TFIIIA; CHAIN: A, D; 5S	KIBUSUMAL KINA GENE; CHAIN:	B, C, E, F;		
Table 5	SEQ FOLD score																												
Tal	score	-	1.00						1.00								1.00								1.00				
V. Comiter	score		-0.07						0.27								0.01								-0.04				
	FSI Blast		8.4e-71						3.4e-37								1.7e-37								3.6e-72				
CINC	AA		430						439								523								570				
TOTATO	AA		266						294								378								406				
i di Airo	CHAIN		A						A								A								¥				
446	FDB ID		1tf6						1tf6								1tf6								1tf6				
Ç	를 의 일 의 의		1451						1451								1451								1451				

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	PDB annotation	INITIATION, ZINC FINGER PROTEIN	COMPLEX (TRANSCRIPTION REGULATION/DNA)	COMPLEX (TRANSCRIPTION	REGULATION/DNA), RNA	POLYMERASE III, 2 TRANSCRIPTION	INITIATION, ZINC FINGER	PROTEIN	COMPLEX (TRANSCRIPTION	REGULATION/DNA)	COMPLEX (TRANSCRIPTION	REGULATION/DNA), RNA	POLYMERASE III, 2	TRANSCRIPTION	INITIATION, ZINC FINGER	PROTEIN	COMPLEX (TRANSCRIPTION	REGULATION/DNA)	COMPLEX (TRANSCRIPTION	REGULATION/DNA), RNA	POLYMERASE III, 2	TRANSCRIPTION	INITIATION, ZINC FINGER	PROTEIN	COMPLEX (TRANSCRIPTION	REGULATION/DNA)	COMPLEX (TRANSCRIPTION	REGULATION/DNA), RNA	POLYMERASE III, 2
	Compound		TFIIIA; CHAIN: A, D; 5S RIBOSOMAL RNA GENE; CHAIN:	B, C, E, F;					TFIIIA; CHAIN: A, D; 5S	KIBOSOMAL KNA GENE; CHAIN:	В, С, Е, Ғ;						TFIIIA; CHAIN: A, D; 5S	RIBOSOMAL RNA GENE; CHAIN:	B, C, E, F;						TFIIIA; CHAIN: A, D; 5S	RIBOSOMAL RNA GENE; CHAIN:	B, C, E, F;		
Table 5	SEQ FOLD score								113.45																				
Ta	PMF		1.00														1.00								1.00				
	Verify score		0.13														0.05								0.30				
	Psi Blast		5.1e-37						3.6e-72								4.8e-69								8.5e-38				
	END		280						596							1	298								009				
	START		434						434								434								462				
	CHAIN		A						А				-				A								V V				
	PDB		146	_				,	1116						-	7,07	ltto								1#6		-1		
	NG EQ		1451				-	,	1451					-		1171	1451							,	1451				

	PDR an
	Compound
ble 5	SEO
Tal	PMF
	Verify
	Psi
	END
	START
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	PDB annotation	TRANSCRIPTION INITIATION, ZINC FINGER PROTEIN	COMPLEX (TRANSCRIPTION REGULATION/DNA) COMPLEX (TRANSCRIPTION REGIT ATTON/DNA) RNA	POLYMERASE III, 2 TRANSCRIPTION	INITIATION, ZINC FINGER PROTEIN	COMPLEX (TRANSCRIPTION REGULATION/DNA) YING-	YANG 1; TRANSCRIPTION	ELEMENT, YY1, ZINC 2	FINGER PROTEIN, DNA-	PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRIPTION	REGULATION/DNA)	COMPLEX (TRANSCRIPTION REGILI ATTON/DNA) VING.	YANG 1; TRANSCRIPTION	INITIATION, INITIATOR	ELEMENT, YY1, ZINC 2	FINGER PROTEIN, DNA-	PROTEIN RECOGNITION, 3	COMPLEX (TRANSCRIPTION	REGULATION/DNA)	COMPLEX (TRANSCRIPTION REGULATION/DNA) YING-
	Compound		TFIIIA; CHAIN: A, D; 5S RIBOSOMAL RNA GENE; CHAIN: B, C, E, F;			YY1; CHAIN: C; ADENO- ASSOCIATED VIRUS P5	INITIATOR ELEMENT DNA; CHAIN: A. B:					YY1; CHAIN: C; ADENO-ASSOCIATED VIRIS PS	INITIATOR ELEMENT DNA;	CHAIN: A, B;					1971: CITABL C. APENIO	ASSOCIATED VIRUS P5
Table 5	SEQ FOLD score																			į
Та	PMF		0.95			96.0						0.99							1 00	1.00
	Verify		-0.21			0.17						-0.01							900	0.00
	Psi Blast		1.7e-33			3.6e-44						8.5e-30							150 20	1.35-30
	END		220			234						234							7,67	707
	START AA		70			125						128							156	001
	CHAIN		A			ပ						ပ)
	PDB ID		1466			1ubd		-				1ubd							1,1hd	TROC
	SEQ NO:		1451			1451						1451							1451	101
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	PDB annotation		YANG 1; TRANSCRIPTION INITIATION INITIATOR	ELEMENT, YY1, ZINC 2	FINGER PROTEIN, DNA-	PROTEIN RECOGNITION, 3	COMPLEX (TRANSCRIPTION	REGULATION/DNA)	COMPLEX (TRANSCRIPTION	REGULATION/DNA) YING-	YANG 1; TRANSCRIPTION	INITIATION, INITIATOR	ELEMENT, YY1, ZINC 2	FINGER PROTEIN, DNA-	PROTEIN RECOGNITION, 3	COMPLEX (TRANSCRIPTION	REGULATION/DNA)	COMPLEX (TRANSCRIPTION	REGULATION/DNA) YING-	YANG 1; TRANSCRIPTION	INITIATION, INITIATOR	ELEMENT, YY1, ZINC 2	FINGER PROTEIN, DNA-	PROTEIN RECOGNITION, 3	COMPLEX (TRANSCRIPTION	REGULATION/DNA)	COMPLEX (TRANSCRIPTION	REGULATION/DNA) YING-	YANG 1; TRANSCRIPTION	INITIATION, INITIATOR	ELEMENT, YY1, ZINC 2	FINGER PROTEIN, DNA-
	Compound		INITIATOR ELEMENT DNA; CHAIN: A. B:						YY1; CHAIN: C; ADENO-	ASSOCIATED VIRUS P5	INITIATOR ELEMENT DNA;	CHAIN: A, B;						YY1; CHAIN: C; ADENO-	ASSOCIATED VIRUS P5	INITIATOR ELEMENT DNA;	CHAIN: A, B;						YY1; CHAIN: C; ADENO-	ASSOCIATED VIRUS P5	INITIATOR ELEMENT DNA;	CHAIN: A, B;		
Table 5	SEQ FOLD	score																														
Ta	PMF								1.00									1.00							• , ,		1.00					
	Verify score								0.20									0.32									0.30					
	Psi Blast								1.1e-47									2.4e-51									6.8e-33					
	END								262	•								346									374					
	START AA						•		158				·					235									273					
	CHAIN								ပ									ပ									ر د			-		
	PDB ID								1ubd		72	 -						lubd									1ubd					
	 	ë Z							1451									1451									1451					

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	Compound PDB annotation	PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULATION/DNA)				
	Co	-	YY1; CHAIN: C; ADENO-ASSOCIATED VIRUS P5 INITIATOR ELEMENT DNA; CHAIN: A, B;	YY1; CHAIN: C; ADENO-ASSOCIATED VIRUS P5 INITIATOR ELEMENT DNA; CHAIN: A, B;	YY1; CHAIN: C; ADENO-ASSOCIATED VIRUS P5 INITIATOR ELEMENT DNA; CHAIN: A, B;	YY1; CHAIN: C; ADENO-
Table 5	SEQ FOLD score			94.56		
Γ_{θ}	PMF		1.00	-	1.00	1.00
1	Verify		0.20		0.42	0.14
	Psi Blast		7.2e-53	3.6e-54	5.1e-35	3.6e-54
	END		430	431	430	486
	START		319	321	329	375
	CHAIN		O	O	O	S
	PDB ID		lubd	lubd	lubd	1ubd
	SEQ B G.		1451	1451	1451	1451

	PDB annotation	REGULATION/DNA) YING-YANG 1; TRANSCRPTION INITIATION, INITIATOR ELEMENT, YY1, ZINC 2 FINGER PROTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGIT ATTON/DNA)	COMPLEX (TRANSCRIPTION REGULATION/DNA) YING-YANG I; TRANSCRIPTION INTIATION INTIATOR ELEMENT, YY1, ZINC 2 FINGER PROTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRIPTION BEGILL ATTOMANA)	COMPLEX (TRANSCRIPTION REGULATION/DNA) YING-YANG 1; TRANSCRIPTION INITIATION INITIATION ELEMENT, YY1, ZINC 2 FINGER PROTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGILL ATION/DNA)	COMPLEX (TRANSCRIPTION REGULATION/DNA) YING-YANG 1; TRANSCRIPTION INITIATION ELEMENT, YY1, ZINC 2
	Compound	ASSOCIATED VIRUS P5 INITIATOR ELEMENT DNA; CHAIN: A, B;	YYI; CHAIN: C; ADENO-ASSOCIATED VIRUS P5 INITIATOR ELEMENT DNA; CHAIN: A, B;	YYI; CHAIN: C; ADENO- ASSOCIATED VIRUS P5 INITIATOR ELEMENT DNA; CHAIN: A, B;	YYI; CHAIN: C; ADENO- ASSOCIATED VIRUS P5 INITIATOR ELEMENT DNA; CHAIN: A, B;
Table 5	SEQ FOLD score				
Ta	PMF		1.00	1.00	1.00
	Verify score		-0.16	0.46	0.20
	Psi Blast		1.2e-34	3.4e-35	1.2e-53
	END		486	514	570
	START		385	413	459
	CHAIN		O	U	S
	PDB		lubd	lubd	1ubd
	SEQ NO:		1451	1451	1451
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	PDB annotation	FINGER PROTEIN, DNA- PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULATION/DNA)	COMPLEX (TRANSCRIPTION REGULATION/DNA) YING- YANG 1; TRANSCRIPTION INITIATION, INITIATOR ELEMENT, YY1, ZINC 2	FINGER PROTEIN, DNA- PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULATION/DNA)	COMPLEX (TRANSCRIPTION REGULATION/DNA) YING- YANG 1; TRANSCRIPTION	INITIATION, INITIATOR ELEMENT, YY1, ZINC 2 FINGER PROTEIN, DNA-	PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULATION/DNA)	COMPLEX (TRANSCRIPTION REGULATION/DNA) YING-YANG 1; TRANSCRIPTION	INITIATION, INITIATOR ELEMENT, YY1, ZINC 2 FINGER PROTEIN DNA-	PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRIPTION	REGULATION/DNA)
	Compound		YY1; CHAIN: C; ADENO- ASSOCIATED VIRUS P5 INITIATOR ELEMENT DNA; CHAIN: A, B;		YY1; CHAIN: C; ADENO- ASSOCIATED VIRUS P5 INITIATOR ELEMENT DNA;	CHAIN: A, B;		YY1; CHAIN: C; ADENO- ASSOCIATED VIRUS P5 INITIATOR ELEMENT DNA;	CHAIN: A, B;		
Table 5	SEQ FOLD score										
Ta	PMF		1.00		1.00			1.00			
	Verify score		0.31		0.22			0.29			
	Psi Blast		1.7e-34		6e-51			3.4e-34			
	END		570		865			598			
	START AA		469		487			497			
ļ	CHAIN		S)			U			
	PDB ID		1ubd		1ubd			1ubd			
	SEQ NO:		1451		1451			1451			

	PDB annotation	COMPLEX (TRANSCRIPTION REGULATION/DNA) YING- YANG 1; TRANSCRIPTION INITIATION, INITIATOR ELEMENT, YY1, ZINC 2 FINGER PROTEIN, DNA- PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULATION/DNA)	COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE- FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA)	COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE- FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA)	COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE- FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA)	COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE- FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA)	COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE-
	Compound	YY1; CHAIN: C; ADENO- ASSOCIATED VIRUS P5 INTITATOR ELEMENT DNA; CHAIN: A, B;	ZINC FINGER PROTEIN GLI1; CHAIN: A; DNA; CHAIN: C, D;	ZINC FINGER PROTEIN GLI1; CHAIN: A; DNA; CHAIN: C, D;	ZINC FINGER PROTEIN GLI1; CHAIN: A; DNA; CHAIN: C, D;	ZINC FINGER PROTEIN GLI1; CHAIN: A; DNA; CHAIN: C, D;	ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D;
Table 5	SEQ FOLD score				96.49		
Tal	PMF	0.57	0.21	1.00		1.00	1.00
	Verify score	-0.46	0.25	0.39		0.17	-0.02
	Psi Blast	1.5e-28	2.4e-63	1e-31	2.4e-65	2.4e-65	3.6e-68
	END AA	178	292	289	320	348	460
	START	72	125	153	181	181	293
	CHAIN	U	∢	4	A	A	A
	PDB ID	Jubd	2gli	2gli	2gli	2gli	2gli
	SEQ El Si	1451	1451	1451	1451	1451	1451

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	PDB annotation	FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA)	COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE- FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA)	COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE- FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA)	COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE- FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA)	COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE- FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA)	COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE- FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA)	COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE- FINGER GLI; GLI, ZINC
	PDI	FINGER GI FINGER, CC BINDING P	COMPLEX (DNA-BINI PROTEIN/DNA) FIVE- FINGER GLI; GLI, ZIN FINGER, COMPLEX (I BINDING PROTEIN/DI	COMPLEX (DNA-BINI PROTEIN/DNA) FIVE- FINGER GLI; GLI, ZIN FINGER, COMPLEX (I BINDING PROTEIN/D)	COMPLEX (DNA-BINI PROTEIN/DNA) FIVE-FINGER GLI; GLI, ZIN FINGER, COMPLEX (I BINDING PROTEIN/D)	COMPLEX (DNA-BIN) PROTEIN/DNA) FIVE- FINGER GI.I; GI.I, ZIN FINGER, COMPLEX (I BINDING PROTEIN/D)	PROTEINE PROTEINE FINGER GI FINGER, CO BINDING P	COMPLEX PROTEIN/I FINGER GI
	Compound		ZINC FINGER PROTEIN GL11; CHAIN: A; DNA; CHAIN: C, D;	ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D;	ZINC FINGER PROTEIN GL11; CHAIN: A; DNA; CHAIN: C, D;	ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D;	ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D;	ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D;
Table 5	SEQ FOLD							
Tal	PMF		1.00	1.00	1.00	1.00	1.00	0.19
	Verify score		0.41	0.22	0.29	0.38	0.31	-0.26
	Psi Blast		1.7e-33	1.2e-68	3.4e-34	1e-33	1.7e-34	5.1e-27
	END		429	572	541	569	009	177
	START AA		301	405	413	441	469	49
	CHAIN		4	4	∢	A	A	А
	PDB ID		2gli	2gli	2gli	2gli	2gli	2gli
	SEQ ID		1451	1451	1451	1451	1451	1451

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	PDB annotation	FINGER, COMPLEX (DNA-BINDING PROTEIN/DNA)	COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE- FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA-	DINDING FROI EIN/DINA)	STRUCTURAL GENOMICS, UNKNOWN FUNCTION HI1434; STRUCTURAL	GENOMICS, UNKNOWN FUNCTION, HYPOTHETICAL	FROIEIN, 2 YBAK	COMPLEX (INHIBITOR/NUCLEASE)	COMPLEX	(INHIBITOR/NUCLEASE), COMPLEX (RI-ANG).	HYDROLASE 2 MOLECULAR	RECOGNITION, EPITOPE	MAPPING, LEUCINE-RICH 3	COMPLEX	(INHIBITOR/NUCLEASE)	COMPLEX	(INHIBITOR/NUCLEASE),	COMPLEX (RI-ANG),	HYDROLASE 2 MOLECULAR RECOGNITION EDITORE	NECOGINITION, EFITOFE
	Compound		ZINC FINGER PROTEIN GLII; CHAIN: A; DNA; CHAIN: C, D;		YBAK; CHAIN: A;			RIBONUCLEASE INHIBITOR; CHAIN: A, D; ANGIOGENIN;	CHAIN: B, E;					RIBONUCLEASE INHIBITOR;	CHAIN: A, D; ANGIOGENIN;	CHAIN: B, E;				
Table 5	SEQ FOLD score																			
Та	PMF		0.24		1.00			1.00						1.00						
	Verify score		-0.16		0.61			0.77						0.43						
	Psi Blast		4.8e-46		1.2e-06			2.4e-32						5.1e-28						
	END		236		116			262						305						
	START		72		13			15					• •	16			_			
	CHAIN		∢		A			¥						A						
1	PDB	;	2glı	;	ngpı			la4y						la4y	 					
S. E.	SEQ NO:	,	1451	,	1456			1459						1459						

	PDB annotation	MAPPING, LEUCINE-RICH 3 REPEATS	COMPLEX (INHIBITOR/NUCLEASE)	(INHIBITORNUCLEASE), COMPLEX (RI-ANG),	HYDROLASE 2 MOLECULAR RECOGNITION, EPITOPE MAPPING, LEUCINE-RICH 3	COMPLEX (NUCLEAR	PROTEIN/RNA) COMPLEX (NUCLEAR PROTEIN/RNA)	RNA,	SNRNP, RIBONUCLEOPROTE IN	COMPLEX (NUCLEAR PROTEIN/RNA) COMPLEX	(NUCLEAR PROTEIN/RNA),	SNRNP, RIBONUCLEOPROTE	COMPLEX (NUCLEAR	PROTEIN/RNA) COMPLEX (NUCLEAR PROTEIN/RNA)	RNA,	SNRNP, RIBONUCLEOPROTE	LIPID TRANSPORT APO A-I; LIPOPROTEIN, LIPID
	Compound		RIBONUCLEASE INHIBITOR; CHAIN: A, D; ANGIOGENIN; CHAIN: B. E:			U2 RNA HAIRPIN IV; CHAIN: Q,	R; U2 A'; CHAIN: A, C; U2 B"; CHAIN: B, D;			U2 RNA HAIRPIN IV; CHAIN: Q, R; U2 A'; CHAIN: A, C; U2 B";	CHAIN: B, D;		U2 RNA HAIRPIN IV; CHAIN: Q,	R; U2 A'; CHAIN: A, C; U2 B"; CHAIN: B, D;			APOLIPOPROTEIN A-I; CHAIN: A, B, C, D;
Table 5	SEQ FOLD	21025									_						77.54
Ta	PMF score		1.00			0.74				69.0			0.53				
	Verify score		0.49			0.15				-0.00			0.20				
	Psi Blast		1.7e-13			1.1e-06				9.6e-10			2.4e-09				1.1e-10
	END		172			178				212			212				447
	START AA		m		***************************************	61				88 88			88				247
	CHAIN		ď			A				Α	-		С				A
5	PDB ID	,	la4y			1a9n				layn			1a9n	-			lavi
010	NO EQ	1450	1429			1459				1439			1459				1459

	PDB annotation		TRANSPORT,	METABOLISM, 2	ATHEROSCLEROSIS, HDL,	LCAT-ACTIVATION	STRUCTURAL PROTEIN	TWO REPEATS OF	SPECTRIN, ALPHA HELICAL	LINKER REGION, 22	TANDEM 3-HELIX COILED-	COILS, STRUCTURAL	PROTEIN	CELL ADHESION LEUCINE	RICH REPEAT, CALCIUM	BINDING, CELL ADHESION	RNA BINDING PROTEIN TAP	(NFX1);	RIBONUCLEOPROTEIN	(RNP, RBD OR RRM) AND	LEUCINE-RICH-REPEAT 2	(LRR)	LIGASE CYCLIN A/CDK2-	ASSOCIATED P45; CYCLIN	A/CDK2-ASSOCIATED P19;	SKP1, SKP2, F-BOX, LRRS,	LEUCINE-RICH REPEATS,	SCF, 2 UBIQUITIN, E3,	UBIQUITIN PROTEIN	LIGASE	CONTRACTILE PROTEIN TRIPLE-HELIX COILED
	Compound		-				ALPHA SPECTRIN; CHAIN: A, B,	౮						INTERNALIN B; CHAIN: A;			NUCLEAR RNA EXPORT	FACTOR 1; CHAIN: A, B;					SKP2; CHAIN: A, C; SKP1;	CHAIN: B, D;						!	HUMAN SKELETAL MUSCLE ALPHA-ACTININ 2; CHAIN: A;
Table 5	SEQ FOLD	score					76.97																								77.32
Ta	PMF													0.89			0.07						0.27								
	Verify score													60.0			-0.20						-0.16								
	Psi Blast	_					2.4e-14							2.4e-06			0.0017						2.4e-10								1.2e-15
	END AA						431							210			126						211								455
	START AA						212							24			47						35								214
	CHAIN ID						A							A			В						A								А
	PDB ID						1cun							1d0b			1fo1						1fs2	-				, .,			1quu
	SEQ ID			- 11	,		1459							1459			1459						1459								1459

	PDB annotation	COIL, CONTRACTILE PROTEIN	TRANSCRIPTION RNA1P; RANGAP; GTPASE-	ACTIVATING PROTEIN FOR	SPII, GTPASE-ACTIVATING PROTEIN, GAP. RNAIP.	RANGAP, LRR, LEUCINE- 2	RICH REPEAT PROTEIN, TWINNING HEMIHEDRAI	TWINNING, 3 MEROHEDRAL	TWINNING, MEROHEDRY	ACETYLATION RNASE	INFIBILOR,	KIBONUCLEASE/ANGIOGEN	IN INTIBITOR A CETY! A TION I BIICINE	RICH REPEATS					TRANSFERASE MITOGEN	KINA SE: TP A NSEEP A SE	MAD KINASE	MAN MANOL,	SEKINE/THREONINE-	PROTEIN KINASE, 2 P38	KINASE RABBIT MUSCLE	PHOSPHORYLASE KINASE;
	Compound		GTPASE-ACTIVATING PROTEIN RNA1_SCHPO; CHAIN: A, B;						A COMPANY OF THE TAXABLE TO CALL	RIBONUCLEASE INHIBITOR;	CHAIR: NOLL;				PHOSPHOTRANSFERASE CAMP-	DEPENDENT PROTEIN KINASE	CATALYTIC SUBUNIT 1CMK 3	(E.C.2./.1.5/) ICMA 4	MAP KINASE P38; CHAIN: NULL;						PHOSPHORYLASE KINASE;	CHAIN: NULL;
Table 5	SEQ FOLD score																									
Ta	PMF		1.00						00	00.1					0.03			1	0.15						-0.14	
	Verify		0.63						0,0	0.38					-0.02			00.0	0.08						90.0	
	Psi Blast		6.8e-20						6	1.2e-29					3.4e-57			17. 10	1./e-/0						6.8e-59	
	END AA		267						6	7.87					504			717	514						207	
	START		10						ľ	,					170			170	6/1						190	
	CHAIN		¥.												ш											
	PDB ID		lyrg						1	uuq7					lcmk			1-20	1528						lphk	
	SEQ NO:		1459						1450	1459					1462			1460	1402						1462	

	PDB annotation	GLYCOGEN METABOLISM, TRANSFERASE, SERINE/THREONINE- PROTEIN, 2 KINASE, ATP- BINDING, CALMODULIN- BINDING		STRUCTURAL PROTEIN TWO REPEATS OF SPECTRIN, ALPHA HELICAL LINKER REGION, 2 2 TANDEM 3-HELIX COILED- COILS, STRUCTURAL PROTEIN	STRUCTURAL PROTEIN	TWO REPEATS OF	SPECTRIN, ALPHA HELICAL	LINKER REGION, 2 2	TANDEM 3-HELIX COILED-	COILS, STRUCTURAL PROTEIN	STRUCTURAL PROTEIN	TWO REPEATS OF	SPECTRIN, ALPHA HELICAL	LINKER REGION, 22	TANDEM 3-HELIX COILED-	COILS, STRUCTURAL	PROTEIN	STRUCTURAL PROTEIN	SPECTRIN, ALPHA HELICAL
	Compound			ALPHA SPECTRIN; CHAIN: A, B, C;	ALPHA SPECTRIN; CHAIN: A, B,	Ú					ALPHA SPECTRIN; CHAIN: A, B,	ပ်						ALPHA SPECTRIN; CHAIN: A, B,	5
Table 5	SEQ FOLD score																		
Tal	PMF			0.13	0.07						0.11							-0.07	
	Verify score			-0.11	90.0						-0.03							0.24	
	Psi Blast			4.8e-05	6e-14		,				9.6e-16							1.2e-15	
	END			699	851						606							928	
	START			523	630	-					069							727	
	CHAIN			A	A						A							A	
	PDB ID		-	1cun	1cun	170					1cun	•						1cun	
	SEQ ID NO:			1465	1465						1465							1465	

	PDB annota		LINKER REGION, TANDEM 3-HELIX	COILS, STRUCTUI	STRUCTURAL PR	SPECTRIN, ALPHA	LINKER REGION,	TANDEM 3-HELLY	COILS, STRUCTUI	PROTEIN	STRUCTURAL PR	TWO REPEATS OF	SPECTRIN, ALPHA	I INITED PECTON
	Compound				ALPHA SPECTRIN; CHAIN: A, B,	ĵ					ALPHA SPECTRIN; CHAIN: A, B,	ర		
Table 5	SEQ	FOLD	21026											
[-	PMF	score			0.11		_				-0.05	,		
	Verify	score		,	0.26						0.19			
	Psi	Blast			3.6e-27						4.8e-16			
	END	AA			981						1073			
	START	ΑA			743						873			
	CHAIN START	О			A						A			_
	PDB	А			cnu						cnu			

MEMBRANE PROTEIN FOUR HA HELICAL S NSEC1; PROTEIN-PROTEIN IA HELICAL COMPLEX, MULTI-SUBUNIT ENDOCYTOSIS/EXOCYTOSI X COILED-TANDEM 3-HELIX COILED-X COILED-FOUR HELICAL-BUNDLE CONTRACTILE PROTEIN ROTEIN ROTEIN HELIX BUNDLE, ALPHA SERINE, CHEMOTAXIS, TRIPLE-HELIX COILED JRAL **JRAL** COIL, CONTRACTILE 1,22 tation COILS, STRUCTURAL SIGNALING PROTEIN LINKER REGION, 22 PROTEIN **PROTEIN** HELIX SYNTAXIN BINDING PROTEIN 1; ALPHA-ACTININ 2; CHAIN: A; HUMAN SKELETAL MUSCLE CHEMOTAXIS PROTEIN I; CHAIN: A; SYNTAXIN 1A; SSO1 PROTEIN; CHAIN: A; METHYL-ACCEPTING CHAIN: A, B; CHAIN: B; -0.15 -0.11 -0.13 -0.06 0.05 0.24 0.08 0.11 2.4e-12 4.8e-11 1.2e-28 3.6e-14 1071 686 859 864 878 711 646 739 ¥ ∢ ¥ В 1qu7 lquu 1dn1 1fio [급 1465 1465 1465 1465 1465 1465 SEQ DO:

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	PDB annotation		SERINE PROTEASE SERINE	PROTEINASE, TRYPSIN,	HYDROLASE	SERINE PROTEASE SERINE	FRO I EINASE, 1 KT FSIN, HYDROLASE	SERINE PROTEINASE	TRYPSIN-LIKE SERINE	PROTEINASE, TETRAMER,	HEPARIN, ALLERGY, 2	ASTHMA	SERINE PROTEASE	PRORENIN CONVERTING	ENZYME (PRECE),	EPIDERMAL GLANDULAR	KALLIKREIN, SERINE	PROTEASE, PROTEIN	MATURATION	SERINE PROTEASE	PRORENIN CONVERTING	ENZYME (PRECE),	EPIDERMAL GLANDULAR	KALLIKREIN, SERINE	PROTEASE, PROTEIN	MATURATION	COMPLEX (BLOOD	COAGULATION/INHIBITOR)	AUTOPROTHROMBIN IIA;	HYDROLASE, SERINE	PROTEINASE), PLASMA
	Compound		TRYPSIN; CHAIN: A, B, C, D;			TRYPSIN; CHAIN: A, B, C, D;		BETA-TRYPTASE; CHAIN: A, B,	C, D;				GLANDULAR KALLIKREIN-13;	CHAIN: A, B;						GLANDULAR KALLIKREIN-13;	CHAIN: A, B;						ACTIVATED PROTEIN C; CHAIN:	C, L; D-PHE-PRO-MAI; CHAIN: P;			
Table 5	SEQ FOLD score		242.91					172.90					216.40														182.46				
[a]	PMF					1.00														1.00	. ,										
	Verify score					0.85										-				06:0											
	Psi Blast		0			0		3.4e-84					7.2e-93							7.2e-93							2.4e-85				
1	END AA		298			298		298					298			-				298							296				
	START AA		64			64		64					64			-											64				
	CHAIN ID		A			A		A					А							A							ပ				
4	PDB ID	,	1a0j			1a0j		1a01					1ao5							1ao5							laut	. —			
	SEQ ID NO:		1471			1471		1471					1471							1471							1471				

	PDB annotation	CALCIUM BINDING, 2 GLYCOPROTEIN, COMPI (BLOOD COAGULATION/INHIBIT	COMPLEX (SERINE PROTEASE/INHIBITOR) TRYPSIN INHIBITOR; COMPLEX (SERINE PROTEASE/INHIBITOR), SERINE PROTEASE, 2 INHIBITOR, COMPLEX, PROTEASE-SUBSTRATE INTERACTIONS, 3 COLLAGEN	SERINE PROTEASE SERI PROTEASE, HYDROLASI COMPLEMENT, FACTOR CATALYTIC 2 TRIAD, SE REGULATION	BLOOD CLOTTING TSV- FIBRINOLYSIS, PLASMINOGEN ACTIVATOR, SERINE PROTEINASE, 2 SNAKE VENOM, COMPLEX (HYDROLASE/INHIBITO BLOOD CLOTTING	SERINE PROTEASE PPE; SERINE PROTEASE, HYDROLASE	COMPLEX (SERINE
	Compound		COLLAGENASE; CHAIN: A, B; ECOTIN; CHAIN: C, D;	COMPLEMENT FACTOR D; CHAIN: NULL;	PLASMINOGEN ACTIVATOR; CHAIN: A, B; GLU-GLY-ARG- CHLOROMETHYLKETONE INHIBITOR; CHAIN: E, F;	ELASTASE; CHAIN: P;	CATHEPSIN G; CHAIN: A;
Table 5	SEQ FOLD		172.65	192.38	198.63	169.32	174.24
Ta	PMF						
	Verify score						
	Psi Blast		3.4e-73	2.4e-87	3.4e-86	9.6e-83	6.8e-74
	END AA		298	296	298	298	297
	START		64	64	64	64	64
	CHAIN ID		∢		A	<u>a</u>	A
	PDB ID		lazz	1bio	Ibqy	1bru	1cgh
	SEQ ID		1471	1471	1471	1471	1471

1																									
	PDB annotation	PROTEASE/INHIBITOR) INFLAMMATION, NHIRITOR SPECIFICITY	SERINE PROTEASE, 2	COMPLEX (SERINE PROTEASE/INHIBITOR)	SERINE PROTEASE	HYDROLASE, SERINE	PROTEASE, DIGESTION, PANCREAS, ZYMOGEN, 2	SIGNAL, MULTIGENE	FAMILY	HYDROLASE/HYDROLASE	INHIBITOR ENTERORINASE, HEAVY CHAIN:	ENTEROKINASE, LIGHT	CHAIN; ENTEROPEPTIDASE,	TRYPSINOGEN	ACTIVATION, 2	HYDROLASE/HYDROLASE	COMPLEX	(PROTEASE/INHIBITOR)	TRYPSIN, COAGULATION	FACTOR XA, CHIMERA,	PROTEASE, PPACK, 2	CHLOROMETHYLKETONE,	COMPLEX	(PROTEASE/INHIBITOR)	
	Compound	PHOSPHONATE INHIBITOR SUC- VAL-PRO-PHEP-(OPH)2; CHAIN: S.	ń		TRYPSIN; CHAIN: NULL;					ENTEROPEPTIDASE; CHAIN: A;	ENTEROPEPTIDASE; CHAIN: B;	PEPTIDE; CHAIN: C;	`				COAGULATION FACTOR XA-	TRYPSIN CHIMERA; CHAIN: A;	D-PHE-PRO-ARG-	CHLOROMETHYLKETONE	(PPACK) WITH CHAIN: I;				HYDROLASE (SERINE PROTEINASE) GAMMA-
Table 5	SEQ FOLD score				234.19					170.43							217.83								175.31
Tak	PMF																								
	Verify score															,									
	Psi Blast				5.1e-99					1.7e-79							1.5e-90								6.8e-81
	END				298					296							298	i i							298
	START AA				64					64							64								54
ļ	CHAIN ID									В							A	i i							A
	PDB ID				1dpo					1ekb							1fxv								1gct
	SEQ ID NO:				1471					1471							1471								1471

	PDB annotation										SERINE PROTEINASE	SERINE PROTEINASE,	GLYCOPROTEIN	HYDROLASE	MICROPLASMINOGEN,	SERINE PROTEASE,	ZYMOGEN, CHYMOTRYPSIN	2 FAMILY, HYDROLASE	GROWTH FACTOR 7S NGF;	GROWTH FACTOR (BETA-	NGF), HYDROLASE - SERINE	PROTEINASE 2 (GAMMA-	NGF), INACTIVE SERINE	PROTEINASE (ALPHA-NGF)	GROWTH FACTOR 7S NGF;	GROWTH FACTOR (BETA-	NGF), HYDROLASE - SERINE	PROTEINASE 2 (GAMMA- NGF), INACTIVE SERINE	
	Compound		*CHYMOTRYPSIN *A (E.C.3.4.21.1) (\$P*H 7.0) 1GCT 3	COMPLEX(PROTEINASE/INHIBI TOR) TRYPSIN (E.C.3.4.21.4)	COMPLEXED WITH INHIBITOR	FROM BITTER 1MCT 3 GOURD	COMPLEX/PROTEINASE/INHIBI	TOR) TRYPSIN (E.C.3.4.21.4)	COMPLEXED WITH INHIBITOR	FROM BITTER 1MCT 3 GOURD 1MCT 4	NEUROPSIN; CHAIN: A, B;			PLASMINOGEN; CHAIN: A, B, C,	Ď;				NERVE GROWTH FACTOR;	CHAIN: A, B, G, X, Y, Z;					NERVE GROWTH FACTOR;	CHAIN: A, B, G, X, Y, Z;			
Table 5	SEQ FOLD	score		243.02							255.96			171.93					183.53						234.25				
Ta	PMF						1.00									,													
	Verify score				_		0.99																						
	Psi Blast			0			0				3.6e-90			1.7e-86					7.2e-79						1.2e-94				
	END			298			298				296			298					798						298				
	START AA			64			64				64			45					73						64				
	CHAIN			A			A				A			Ą					A						G				
	PDB ED			1mct			1mct				1npm		ļ	lqrz					1sgf						1sgf				
	SEQ ED	: Se		1471			1471				1471			1471					1471						1471				

	PDB annotation	PROTEINASE (ALPHA-NGF)	GROWTH FACTOR 7S NGF;	GROW IN FACTOR (BETA- NGF), HYDROLASE - SERINE	PROTEINASE 2 (GAMMA-	NGF), INACTIVE SERINE	PROTEINASE (ALPHA-NGF)	COMPLEX (SERINE	TRYPSIN INHIBITOR:	SERINE PROTEASE,	INHIBITOR, COMPLEX,	METAL BINDING SITES, 2	PROTEIN ENGINEERING,	PROTEASE-SUBSTRATE	INTERACTIONS, 3	METALLOPROTEINS	COMPLEX (SERINE	TRYPSIN INHIBITOR:	CED INE DOOTE A CE	SEMINE INCIENSE,	INTIBILOR, COMPLEA,	MEIAL BINDING SILES, 2	PROTEIN ENGINEERING,	PROTEASE-SUBSTRATE	INTERACTIONS, 3	METALLOPROTEINS		
	Compound		NERVE GROWTH FACTOR;	CITALIN: A, B, G, A, I, Z,				ECOTIN; CHAIN: A; ANIONIC									ECOTIN; CHAIN: A; ANIONIC	inti out, citatin D,									HYDROLASE(SERINE PROTEINASE) TONIN (E.C.	NUMBER NOT ASSIGNED) 11ON 4
Table 5	SEQ FOLD score							224.62																	·		210.31	
Tal	PMF		1.00														1.00											
	Verify		68.0														98.0											
	Psi Blast		1.2e-94					0									0										1.1e-91	
	END		298					298									298										298	
	START AA		64					64									64										64	
	CHAIN		Ð					M									В											
	PDB		1sgf					lslw									1slw										Iton	
	S S S S S S		1471					1471									1471										1471	

	PDB annotation						SERINE PROTEASE
	Compound	HYDROLASE(SERINE PROTEINASE) TONIN (E.C. NUMBER NOT ASSIGNED) 1TON 4	HYDROLASE (SERINE PROTEINASE) TRYPSIN (E.C.3.4.21.4) COMPLEXED WITH THE INHIBITOR 1TRN 3 DIISOPROPYL-FLUOROPHOSPHOFLUORIDATE (DFP) 1TRN 4 HUMAN TRYPSIN, DFP INHIBITED 1TRN 6	HYDROLASE (SERINE PROTEINASE) TRYPSIN (E.C.3.4.21.4) COMPLEXED WITH THE INHIBITOR 1TRN 3 DIISOPROPYL. FLUOROPHOSPHOFLUORIDATE (DFP) 1TRN 4 HUMAN TRYPSIN, DFP INHIBITED 1TRN 6	HYDROLASE(SERINE PROTEINASE) TRYPSIN (E.C.3.4.21.4) COMPLEXED WITH BENZAMIDINE INHIBITOR 2TBS	HYDROLASE(SERINE PROTEINASE) TRYPSIN (E.C.3.4.21.4) COMPLEXED WITH BENZAMIDINE INHIBITOR 2TBS	BETA TRYPSIN; CHAIN: NULL;
Table 5	SEQ FOLD score		234.44			235.83	235.23
Ta	PMF score	1.00		1.00	1.00		
	Verify score	0.87		0.92	0.85		
	Psi Blast	1.1e-91	0	0	0	0	1.7e-
ļ	END	298	298	298	296	298	298
	START AA	67	64	64	64	64	64
	CHAIN		∢	A			
	PDB ID	lton	1tm	1fm	2tbs	2tbs	5ptp
	S E S	1471	1471	1471	1471	1471	1471

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	PDB annotation	HYDROLASE, SERINE PROTEASE, DIGESTION, PANCREAS, 2 ZYMOGEN, SIGNAT	SERINE PROTEASE HYDROLASE, SERINE PROTEASE, DIGESTION, PANCREAS, 2 ZYMOGEN, SIGNAL		COMPLEX (ZINC FINGER/DNA) COMPLEX (ZINC FINGER/DNA) ZINC	FINGER, DNA-BINDING PROTEIN	COMPLEX (ZINC FINGER/DNA) COMPLEY	(ZINC FINGER/DNA), ZINC FINGER, DNA-BINDING	COMPLEX (ZINC	FINGER/DNA) COMPLEX	(ZINC FINGER/DNA), ZINC	FINGER, DINA-BINDING PROTEIN	COMPLEX (ZINC	FINGER/DNA) COMPLEX	(ZINC FINGER/DNA), ZINC	FINGER, DNA-BINDING	COMPLEX (ZINC
	Compound		BETA TRYPSIN; CHAIN: NULL;		QGSR ZINC FINGER PEPTIDE; CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING	SITE; CHAIN: B, C;	QGSR ZINC FINGER PEPTIDE; CHAIN: A; DUPLEX	OLIGONUCLEOTIDE BINDING SITE; CHAIN: B, C;	QGSR ZINC FINGER PEPTIDE;	CHAIN: A; DUPLEX	OLIGONUCLEOTIDE BINDING STEF. CHAIN: P. C.	orre, cumin. D, C,	QGSR ZINC FINGER PEPTIDE;	CHAIN: A; DUPLEX	OLIGONUCLEOTIDE BINDING	SITE; CHAIN: B, C;	QGSR ZINC FINGER PEPTIDE;
Table 5	SEQ FOLD score												70.55		<u> </u>	***************************************	
Ta	PMF		1.00		0.58		96.0		1.00								0.81
	Verify		0.93		-0.06		0.36		0.18								0.08
	Psi Blast	100	1.7e- 100		3.4e-15		1.2e-28		3.4e-31				3.4e-31			_	1.7e-27
	END		298		412	27	440		468				470				499
	START AA		64		349	720	520		386				386				416
1 24	CHAIN ID				V	<	——		A				A				A
44	PDB ID		5ptp		lalh	75	14111		lalh			-	lain				lalh
010	NÖ E Ö		1471		14/8	1778	0/#1		1478				14/0			· · ·	1478

	PDB annotation		FINGER/DNA) COMPLEX (ZINC FINGER/DNA), ZINC FINGER, DNA-BINDING PROTEIN	COMPLEX (ZINC FINGER/DNA) COMPLEX (ZINC FINGER/DNA), ZINC FINGER, DNA-BINDING PROTEIN		COMPLEX (ZINC	FINGER/DNA) ZINC FINGER, PROTEIN-DNA	INTERACTION, PROTEIN	DESIGN, 2 CRYSTAL	STRUCTURE, COMPLEX (ZINC FINGER/DNA)	COMPLEX (ZINC FINGER PINGER	PROTEIN-DNA	INTERACTION, PROTEIN	DESIGN, 2 CRYSTAL	STRUCTURE, COMPLEX	(ZINC FINGER/DNA)	COMPLEX (ZINC FINGER/DNA) ZINC FINGER,
	Compound		CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE; CHAIN: B, C;	QGSR ZINC FINGER PEPTIDE; CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE; CHAIN: B, C;	DNA-BINDING PROTEIN HUMAN ENHANCER-BINDING PROTEIN MBP-1 MUTANT WITH CYS 11 1BBO 3 REPLACED BY ABU (C11ABU) (NMR, 60 STRUCTURES) 1BBO 4	DNA; CHAIN: A, B, D, E;	CONSENSUS ZINC FINGER PROTEIN: CHAIN: C. F. G:				DNA; CHAIN: A, B, D, E;	PROTEIN; CHAIN; C, F, G;					DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER
Table 5	SEQ FOLD	score															
Та	PMF			0.22	0.58	0.57					1.00						1.00
	Verify score			-0.36	-0.27	-0.27					0.26						0.23
	Psi Blast			8.5e-19	4.8e-16	3.4e-28					6.8e-45						1e-47
	END AA			504	471	412					440						468
	START AA			444	418	348					354				_		385
	CHAIN			A		S					C						S
	PDB ID			lalh	1bbo	1mey					1mey						1mey
	SEQ ID	NO:		1478	1478	1478					1478						1478

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	PDB annotation	PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX	COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX	CLINC FUNGERDINA) COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX	(ZINC FINGERDNA) COMPLEX (ZINC FINGER, DNA PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA)	COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL
	Compound	PROTEIN; CHAIN: C, F, G;	DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G;	DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G;	DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G;	DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G;
Table 5	SEQ FOLD score		65.65			
Ta	PMF score			0.95	0.16	69.0
	Verify score			0.02	-0.30	0.44
	Psi Blast		1e-47	5.1e-47	6.8e-32	3.4e-11
	END AA		469	498	504	412
	START AA		385	415	443	383
	CHAIN		O	U	O	Ð
	PDB		Imey	lmey	Imey	Imey
3	NO E		1478	1478	1478	1478

	PDB annotation		STRUCTURE, COMPLEX (ZINC FINGER/DNA)	COMPLEX (ZINC	FINGER/DNA) ZINC FINGER,	PROTEIN-DNA	INTERACTION, PROTEIN	DESIGN, 2 CRYSTAL	STRUCTURE, COMPLEX (ZINC FINGER (DNA)	ZINC FINGER	TRANSCRIPTION FACTOR	SP1; ZINC FINGER.	TRANSCRIPTION	ACTIVATION, SP1	COMPLEX (TRANSCRIPTION	KEGULAIION/DINA) IFIIIA;	SS GENE; NMR, TFIIIA,	PROTEIN, DNA,	TRANSCRIPTION FACTOR,	SS RNA 2 GENE, DNA	BINDING PROTEIN, ZINC	FINGER, COMPLEX 3	(TRANSCRIPTION	REGULATION/DNA)	COMPLEX (TRANSCRIPTION	REGULATION/DNA) TFIIIA;	SS GENE; NMR, TFIIIA,	PROTEIN, DNA,	TRANSCRIPTION FACTOR,	5S RNA 2 GENE, DNA	BINDING PROTEIN, ZINC
	Compound			DNA; CHAIN: A, B, D, E;	CONSENSUS ZINC FINGER	PROTEIN; CHAIN: C, F, G;				SP1F2; CHAIN: NULL;					TRANSCRIPTION FACTOR IIIA;	CHAIN: A; 33 KINA GENE;	CHAIN: E, F;								TRANSCRIPTION FACTOR IIIA;	CHAIN: A; 5S RNA GENE;	CHAIN: E, F;				
Table 5	SEQ FOLD	score																													
Tat	PMF			0.45						0.58					0.17										0.77						
	Verify score			-0.33						0.05					0.20										0.26						
	Psi Blast			1e-12				***************************************		6.8e-09					1.7e-15						•				8.5e-23						
	END AA			468						416					412										440						
	START AA			441						386	•••				348										355						
	CHAIN			ß											A										A						
	PDB ID			1mey						1sn2	4				1tf3										11f3						
	SEQ EL			1478						1478					1478										1478						

	PDB annotation	FINGER, COMPLEX 3 (TRANSCRIPTION REGULATION/DNA)	COMPLEX (TRANSCRIPTION REGULATION/DNA) TFIIIA; 5S GENE; NMR, TFIIIA,	TRANSCRIPTION FACTOR, 5S RNA 2 GENE, DNA	BINDING PROTEIN, ZINC FINGER, COMPLEX 3	(TRANSCRIPTION REGULATION/DNA)	COMPLEX (TRANSCRIPTION REGILATION/DNA) TEITIA:	SS GENE; NMR, TFIIIA,	PROTEIN, DNA,	TRANSCRIPTION FACTOR,	5S RNA 2 GENE, DNA	BINDING PROTEIN, ZINC	(TRANSCRIPTION	REGULATION/DNA)	COMPLEX (TRANSCRIPTION REGULATION/DNA)	COMPLEX (TRANSCRIPTION	REGULATION/DNA), RNA	POLYMERASE III, 2	TRANSCRIPTION	INITIATION, ZINC FINGER PROTEIN
	Compound		TRANSCRIPTION FACTOR IIIA; CHAIN: A; 5S RNA GENE; CHAIN: E, F;				TRANSCRIPTION FACTOR IIIA; CHAIN: A: 5S RNA GENE:	CHAIN: E, F;							TFIIIA; CHAIN: A, D; 5S RIBOSOMAL RNA GENE: CHAIN:	B, C, E, F;				
Table 5	SEQ FOLD score														71.55					
Ta	PMF		0.35				0.03													
	Verify score		-0.25				-0.23													
	Psi Blast		6.8e-20				1.2e-13								1.7e-37					
	END		499				503								499					
	START		416				444	_	-						325					
	CHAIN	,	A				A								А					
	PDB ID		1tf3				143								1tf6					

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	PDB annotation	COMPLEX (TRANSCRIPTION REGULATION/DNA) COMPLEX (TRANSCRIPTION REGULATION/DNA), RNA POLYMERASE III, 2 TRANSCRIPTION INITIATION, ZINC FINGER PROTEIN	COMPLEX (TRANSCRIPTION REGULATION/DNA) YING-YANG 1; TRANSCRIPTION INITIATOR ELEMENT, YY1, ZINC 2 FINGER PROTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULATION/DNA)	COMPLEX (TRANSCRIPTION REGULATION/DNA) YING-YANG 1; TRANSCRIPTION INITIATION INITIATOR ELEMENT, YY1, ZINC 2 FINGER PROTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULATION/DNA)	COMPLEX (TRANSCRIPTION REGULATION/DNA) YING- YANG 1; TRANSCRIPTION INITIATION, INITIATOR ELEMENT, YY1, ZINC 2			
	Compound	TFIIIA; CHAIN: A, D; 5S RIBOSOMAL RNA GENE; CHAIN: B, C, E, F;	YY1; CHAIN: C; ADENO- ASSOCIATED VIRUS P5 INITIATOR ELEMENT DNA; CHAIN: A, B;	YY1; CHAIN: C; ADENO- ASSOCIATED VIRUS P5 INITIATOR ELEMENT DNA; CHAIN: A, B;	YYI; CHAIN: C; ADENO- ASSOCIATED VIRUS P5 INITIATOR ELEMENT DNA; CHAIN: A, B;			
Table 5	SEQ FOLD score							
Tal	PMF	0.50	09.0	1.00	66:0			
	Verify score	-0:12	0.07	60:00	-0.42			
	Psi Blast	1.7e-37	5.1e-20	4.8e-26	5.1e-29			
	END	105	412	468	440			
	START	355	351	359	361			
	CHAIN ID	¥	O	ن ن	ت ت			
	PDB ID	14f6	lubd	lubd	1ubd			
	SEQ NO:	1478	1478	1478	1478			

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	PDB annotation	FINGER PROTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGILL ATTOMONA)	COMPLEX (TRANSCRIPTION REGULATION/DNA) YING- YANG 1; TRANSCRIPTION INITIATION, INITIATOR	ELEMENT, YY1, ZINC 2 FINGER PROTEIN, DNA- PROTEIN RECOGNITION, 3	COMPLEX (TRANSCRIPTION REGULATION/DNA)	COMPLEX (TRANSCRIPTION	KEGULATION/DNA) YING- YANG 1; TRANSCRIPTION	INITIATION, INITIATOR	ELEMENT, YY1, ZINC 2	FINGER PROTEIN, DNA-	FROI EIN KECOGNI I ION, 3	REGULATION/DNA)	COMPLEX (TRANSCRIPTION	REGULATION/DNA) YING-	INITIATION INITIATOR	ELEMENT, YY1, ZINC 2	FINGER PROTEIN, DNA-	PROTEIN RECOGNITION, 3	COMPLEX (TRANSCRIPTION	(NEGOLATION/DINA)
	Compound		YYI; CHAIN: C; ADENO- ASSOCIATED VIRUS P5 INITIATOR ELEMENT DNA; CHAIN: A, B;			YY1; CHAIN: C; ADENO-	ASSOCIATED VIKUS PS INITIATOR ELEMENT DNA;	CHAIN: A, B;					YY1; CHAIN: C; ADENO-	ASSOCIATED VIRUS P5 INITIATOR FI FMENT DNA:	CHAIN: A, B;					
Table 5	SEQ FOLD score		75.80												•					
Ta	PMF					1.00							0.57							
	Verify scoré					-0.04							-0.10							
	Psi Blast		3.4e-34			3.4e-34							1.7e-25							
	END		499			498							504							
	START AA		387			390							423							
	CHAIN ID		O			S							ပ							
	PDB		lubd	,		1npq					_		1nbd							
	SEQ U NO:		1478			1478							1478							

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	PDB annotation	TRANSCRIPTION REGULATION TRANSCRIPTION REGULATION, ADRI, ZINC FINGER, NMR	TRANSCRIPTION REGULATION TRANSCRIPTION REGULATION, ADRI, ZINC FINGER, NMR	COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE- FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA)	COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE- FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA)	COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE- FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA- BINDING PROTEIN/DNA)	COMPLEX (ZINC FINGER/DNA) COMPLEX (ZINC FINGER/DNA), ZINC FINGER, DNA-BINDING PROTEIN
	Compound	ADR1; CHAIN: NULL;	ADR1; CHAIN: NULL;	ZINC FINGER PROTEIN GL11; CHAIN: A; DNA; CHAIN: C, D;	ZINC FINGER PROTEIN GLI1; CHAIN: A; DNA; CHAIN: C, D;	ZINC FINGER PROTEIN GLI1; CHAIN: A; DNA; CHAIN: C, D;	QGSR ZINC FINGER PEPTIDE; CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE; CHAIN: B, C;
Table 5	SEQ FOLD score				74.47		
Tal	PMF	66.0	0.24	0.99		66:0	1.00
	Verify score	-0.18	-0.02	0.21		0.27	0.35
	Psi Blast	16-15	3.4e-15	1.2e-33	1.7e-36	1.7e-36	2.4e-35
	END	470	501	467	200	499	378
	START AA	418	444	350	356	359	294
	CHAIN			A	A	A	A
	PDB ID	2adr	2adr	2gli	2gli	2gli	lalh
	SEQ ID NO:	1478	1478	1478	1478	1478	1488

PDB annotation	COMPLEX (ZINC FINGER/DNA) COMPLEX (ZINC FINGER/DNA), ZINC FINGER, DNA-BINDING	PROTEIN COMPLEX (ZINC FINGER/DNA) COMPLEX (ZINC FINGER/DNA), ZINC FINGER, DNA-BINDING	PROTEIN COMPLEX (ZINC FINGER/DNA) COMPLEX (ZINC FINGER/DNA), ZINC FINGER, DNA-BINDING	PROTEIN TRANSFERASE DINUCLEOTIDE-BINDING MOTIF, PHOSPHORIBOSYL	TRANSFERASE COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX	(ZINC FINGER/DNA) COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN 2 CRYSTAI
Compound	QGSR ZINC FINGER PEPTIDE; CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE; CHAIN: B, C;	QGSR ZINC FINGER PEPTIDE; CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE; CHAIN: B, C;	QGSR ZINC FINGER PEPTIDE; CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE; CHAIN: B, C;	NICOTINATE MONONUCLEOTIDE:5,6- CHAIN: A;	DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G;	DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G;
SEQ FOLD	87.16				94.84	
PMF		1.00	1.00	-0.14		1.00
Verify score		0.47	0.17	0.03		0.29
Psi Blast	2.4e-35	1.2e-29	5.1e-27	1.2e-09	1.4e-51	1.46-51
END AA	380	378	395	291	379	378
STARI	294	296	324	32	293	295
CHAIN	A	Ą	¥	A	U	U
TUB ID	laih	lath	la1h	1d0s	1mey	Imey
Ž A Š	1488	1488	1488	1488	1488	1488
	FDB CLIAIN START END Psi Verify PMF SEQ Compound ID ID AA AA Blast score FOLD	TDB CHAIN START END Psi Verify PMF SEQ Compound Bast score score FOLD score 1a1h A 294 380 2.4e-35 CHAIN: A; DUPLEX CHAIN: B, C; CHAIN: B, C;	TDB CHAIN STAKT END Psi Verify PMF SEQ Compound AA Blast score fOLD score FOLD Store 1a1h A 294 380 2.4e-35 1a1h A 296 378 1.2e-29 0.47 1.00 QGSR ZINC FINGER PEPTIDE; CHAIN: B, C; CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE; CHAIN: B, C; CHAIN: CHAIN: B, C; CHAIN:	141h A 294 380 2.46-35 Score FOLD CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE; CHAIN: B, C; CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE; CHAIN: B, C; CHAIN: B, C	141h A 294 380 2.4e-35 Score FOLD Score FOLD FOLD Score FOLD FOLD FOLD Score FOLD FO	14Th A 294 380 2.46-35 Score FOLD Score CHAIN: A; DUPLEX CHAIN: B, C; CHAIN: CHAIN: CHAIN: C, E, G; CHAIN: C, E, G; CHAIN: C, E, G; CHAIN: C, E, G; CHAIN: C, E, C,

:	PDB annotation		STRUCTURE, COMPLEX (ZINC FINGER/DNA)	COMPLEX (ZINC	FINGER/DNA) ZINC FINGER,	PROTEIN-DNA	INTERACTION, PROTEIN	DESIGN, 2 CRYSTAL	STRUCTURE, COMPLEX	COMPLEX (TRANSCRIPTION	REGIT ATTON/DNA) TEITIA:	5S GENE; NMR. TFIIIA.	PROTEIN, DNA,	TRANSCRIPTION FACTOR,	5S RNA 2 GENE, DNA	BINDING PROTEIN, ZINC	FINGER, COMPLEX 3	(TRANSCRIPTION	REGULATION/DNA)	COMPLEX (TRANSCRIPTION	REGULATION/DNA)	COMPLEX (TRANSCRIPTION	REGULATION/DNA), RNA	POLYMERASE III, 2	TRANSCRIPTION	INITIATION, ZINC FINGER	PROTEIN	COMPLEX (TRANSCRIPTION	KEGULATION/DNA) YING-	YANG I; IRANSCRIPTION INITIATION, INITIATOR
	Compound		·	DNA: CHAIN: A B D E.	CONSENSUS ZINC FINGER	PROTEIN; CHAIN: C, F, G;				TRANSCRIPTION FACTOR IIIA:	CHAIN: A: 5S RNA GENE:	CHAIN: E, F;								TFIIIA; CHAIN: A, D; 5S	RIBOSOMAL RNA GENE; CHAIN:	B, C, E, F;					Order O retired 1771	YYI; CHAIN: C; ADENO-	ASSOCIATED VIRUS PS	INITIATOK ELEMENT DNA; CHAIN: A, B;
Table 5	SEQ FOLD	score								73.75										61.08							000	80.80		
Ta	PMF			1.00	•																									
	Verify score			0.39																										
	Psi Blast			1e-43	!					5.1e-21			_							le-25							10, 21	0.8e-31		
	END AA			398	,					382										398							07.0	5/9		
	START			323						293										240	-						0),	607		
	CHAIN			C						A										Ą							C	ی		
	PDB ID			1mey						1tf3	-									1tf6							1.1.1	panı		
į	SEQ	Ö.		1488						1488										1488							1400	1488		

	PDB annotation		ELEMENT, YY1, ZINC 2 FINGER PROTEIN, DNA-	PROTEIN RECOGNITION, 3	COMPLEX (TRANSCRIPTION PEGIT A TYONIAN)		S COMFLEA (TRANSCRIFTION REGULATION/DNA) YING-		FI FMENT VV1 ZNC 2	FINGER PROTEIN, DNA-	PROTEIN RECOGNITION, 3	COMPLEX (TRANSCRIPTION					INITIATION, INITIATOR	ELEMENT, YY1, ZINC 2	FINGER PROTEIN, DNA-	PROTEIN RECOGNITION, 3	COMPLEX (TRANSCRIPTION				FINGER GLI; GLI, ZINC	FINGER, COMPLEX (DNA-			
	Compound					YY1: CHAIN: C: ADFNO	ASSOCIATED VIRUS P5	INITIATOR ELEMENT DNA; CHAIN: A R:	, T. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1.					YY1; CHAIN: C; ADENO-	ASSOCIATED VIRUS PS	INITIATIOR ELEMENT DNA;	CHAIN: A, B;						ZINC FINGER PROTEIN GLII;	CHAIN: A; DNA; CHAIN: C, D;	•			ZINC FINGER PROTEIN GI 11	(117)
Table 5	SEQ FOLD	score																					78.30						_
Ta	PMF score					1.00					_		6	00:1														1.00	-
	Verify score					0.30							110	0.11														0.38	
	Psi Blast					6.8e-31							1 7, 20	1.26-28								2 40.21	2.46-31					7.4e-31	
	END AA					378			•				300	390								280	000					2/8	
	START					296		-					301	100								237	/ (77				1	7/1	
, at 1 in	CHAIN					ر ر)								A	47					۲	
4.44	EDE EDE					1ubd		_	-				111hd							•		Joli						- g ₁₁	
000	E C	ë.	-			1488							1488	2								1488			·		1400		

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	PDB annotation		FINGER, COMPLEX (DNA-BINDING PROTEIN/DNA)	COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE-	FINGER GLI; GLI, ZINC FINGER, COMPLEX (DNA-	BINDING PROTEIN/DNA)	COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE.	FINGER GLI, GLI, ZINC	FINGER, COMPLEX (DNA-	BINDING FROI EIN/DINA)	COMPLEX (TRANSCRIPTION REGITT ATTOM/DIAM)	GABPALPHA; GABPBETA1;	COMPLEX (TRANSCRIPTION	REGULATION/DNA), DNA-	BINDING, 2 NUCLEAR	PROTEIN, ETS DOMAIN,	ANKYRIN REPEATS,	TRANSCRIPTION 3 FACTOR	COMPLEX (TRANSCRIPTION	(KEGULAIION/DNA)	GABFALFHA; GABFBE1AI;	COMPLEX (TRANSCRIPTION	KEGULATION/DNA), DNA-	BINDING, 2 NUCLEAR	PROTEIN, ETS DOMAIN,	ANKYRIN REPEATS,	INDIANGUITION OF THE TOTAL OF
	Compound			ZINC FINGER PROTEIN GLI1; CHAIN: A; DNA; CHAIN: C, D;			ZINC FINGER PROTEIN GLII; CHAIN: A: DNA: CHAIN: C D:				GA BINDING PROTEIN ALPHA; CHAIN: A: GA BINDING	PROTEIN BETA 1; CHAIN: B;	DNA; CHAIN: D, E;						GA BINDING PROTEIN ALPHA;	CHAIN: A; GA BINDING	PROTEIN BETA I; CHAIN: B;	DNA; CHAIN: D, E;					
Table 5	SEQ	score									53.03																
Ta	PMF	SCOIC		1.00			1.00												1.00								
	Verify	Score		0.52			0.04												0.88								
	Psi Blast	Dida		3.4e-26			1.7e-26				3.4e-33								3.4e-33								
	END	AA		377			398				224								224								
	START	WW.	:	295			313				111								114								
!	CHAIN	<u> </u>		A			Ą				A								A								
	PDB	i i		2gli			2gli	***			1awc								1awc								
,	SEQ	g Ö		1488			1488				1489								1489								

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	PDB annotation		TRANSCRIPTION REGULATION	COMPLEX (TRANSCRIPTION FACTOR/DNA)	COMPLEX (TRANSCRIPTION FACTOR/DNA)	COMPLEX (TRANSCRIPTION REGULATING/DNA) PU.1; COMPLEX (TRANSCRIPTION REGULATING/DNA), ONCOGENE, 2 TRANSFORMING PROTEIN, DNA-BINDING, ACTIVATOR, 3 NUCLEAR PROTEIN	COMPLEX (TRANSCRIPTION REGULATING/DNA) PU.1; COMPLEX (TRANSCRIPTION REGULATING/DNA), ONCOGENE, 2 TRANSFORMING PROTEIN, DNA-BINDING, ACTIVATOR, 3 NUCLEAR PROTEIN	COMPLEX (NUCLEOCAPSID PROTEIN/DNA) (12-53)NCP7; COMPLEX (NUCLEOCAPSID PROTEIN/DNA), NUCLEIC ACID, 2 RETROVIRUS,
	Compound		MURINE ETS-1 TRANSCRIPTION FACTOR; 1ETC 4 CHAIN: NULL; 1ETC 5	FLI-1; 1FLI 5 CHAIN: A; 1FLI 6 DNA 1FLI 10 CHAIN: B, C; 1FLI 12	FLI-1; 1FLI 5 CHAIN: A; 1FLI 6 DNA 1FLI 10 CHAIN: B, C; 1FLI 12	DNA (16 BASE PAIRS); CHAIN: A, B, C, D; TRANSCRIPTION FACTOR PU.1; CHAIN: E, F;	DNA (16 BASE PAIRS); CHAIN: A, B, C, D; TRANSCRIPTION FACTOR PU.1; CHAIN: E, F;	DNA (ACGCC); CHAIN: D; NUCLEOCAPSID PROTEIN 7; CHAIN: A;
Table 5	SEQ FOLD	score		59.75		92.89		
Tal	PMF score		0.99		96.0		1.00	0.45
	Verify score		0.47		0.27		0.86	-0.57
	Psi Blast		6.8e-36	3.4e-32	3.4e-32	8.5e-32	8.5e-32	0.00024
	END AA		220	204	203	197	197	129
	START AA		114	106	114	110	114	106
	CHAIN ID			A	A	я	ш	A
	PDB ID		letc	1fli	1fli] bne	1pue	1bj6
	SEQ ID	NO.	1489	1489	1489	1489	1489	1495

	PDB annotation	VIRUS MORPHOGENESIS, ZINC FINGER			PROTEIN/DNA HOMEODOMAIN, DNA, COMPLEX, DNA-BINDING PROTEIN, PROTEIN/DNA	PROTEIN/DNA HOMEODOMAIN, DNA, COMPLEX, DNA-BINDING PROTEIN, PROTEIN/DNA	TRANSFERASE DINUCLEOTIDE-BINDING MOTIF, PHOSPHORIBOSYL TRANSFERASE	
	Compound		DNA-BINDING PROTEIN ANTENNAPEDIA PROTEIN (HOMEODOMAIN) MUTANT WITH CYS 39 1AHD 3 REPLACED BY SER (C39S) COMPLEX WITH DNA (NMR, 1AHD 4 16 STRUCTURES) 1AHD 5	DNA-BINDING PROTEIN ANTENNAPEDIA PROTEIN (HOMEODOMAIN) MUTANT WITH CYS 39 1AHD 3 REPLACED BY SER (C39S) COMPLEX WITH DNA (NMR, 1AHD 4 16 STRUCTURES) 1AHD 5	HOMEOBOX PROTEIN HOX-B1; CHAIN: A; PBX1; CHAIN: B; DNA CHAIN: D; DNA CHAIN: E;	HOMEOBOX PROTEIN HOX-B1; CHAIN: A; PBX1; CHAIN: B; DNA CHAIN: D; DNA CHAIN: E;	NICOTINATE MONONUCLEOTIDE:5,6- CHAIN: A;	DNA-BINDING FUSHI TARAZU PROTEIN (HOMEODOMAIN)
Table 5	SEQ FOLD score			66.86	59.01			59.28
Ta	PMF		0.99			1.00	-0.19	
	Verify score		-0.14			0.01	0.58	
	Psi Blast	-	1.7e-35	1.7e-35	8.5e-28	8.5e-28	4.4e-12	1e-30
	END		302	307	298	298	243	309
	START AA		237	237	231	241	71	235
	CHAIN		d	Д	А	А	А	
	PDB ID		lahd	lahd	1572	1572	1d0s	1ftz
	S B S		1497	1497	1497	1497	1497	1497

	PDB annotation			COMPLEX (HOMEODOMAIN/DNA) VND/NK-2 HOMEODOMAIN,	VENTRAL NERVOUS SYSTEM HOMEODOMAIN, HOMFOROY DNA-RINDING	PROTEIN, EMBRYONIC 2 DEVELORMENT COMPLEY	(HOMEODOMAIN/DNA)	COMPLEX	(HOMEODOMAIN/DNA) VND/NK-2 HOMEODOMAIN,	VENTRAL NERVOUS	SYSTEM HOMEODOMAIN,	HOMEOBOX, DNA-BINDING	PROTEIN, EMBRYONIC 2	DEVELOPMENT, COMPLEX (HOMEODOMAIN/DNA)	OUTER MEMBRANE	PROTEIN OSMOPORIN;	OUTER MEMBRANE	PROTEIN, NON-SPECIFIC	PORIN, OSMOPORIN, 2	BETA-BARREL,	TRANSMEMBRANE	DNA-BINDING PROTEIN HELIX-TURN-HELIX, DNA-
	Compound	(NMR, 20 STRUCTURES) 1FTZ 3	DNA-BINDING FUSHI TARAZU PROTEIN (HOMEODOMAIN) (NMR, 20 STRUCTURES) IFTZ 3	HOMEOBOX PROTEIN VND; CHAIN: P; DNA; CHAIN: A, B;				HOMEOBOX PROTEIN VND;	CHAIN: F; DNA; CHAIN: A, B;						OMPK36; CHAIN: A, B, C;							HOMEOBOX VENTRAL NERVOUS SYSTEM DEFECTIVE
Table 5	SEQ FOLD score			55.18																		54.12
Ta	PMF		86.0					0.99				•			-0.20							
	Verify score		-0.04					-0.33							0.65							
	Psi Blast		1e-30	1.5e-17				1.5e-17							1.5e-08							6.8e-17
	END		296	307				302			.,1-				244							307
	START AA		237	229				234							77							226
	CHAIN			<u>a</u>				Ь							A							A
	PDB		1 ffz	1nk2				1nk2							losm							lqry
	SEQ NO:		1497	1497	****			1497							1497							1497
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	PDB annotation		BINDING PROTEIN	DNA-BINDING PROTEIN HELIX-TURN-HELIX, DNA- BINDING PROTEIN					COMPLEX (DNA-BINDING PROTEIN/DNA) HD;	HOMEODOMAIN, COMPLEX (DNA-BINDING PROTEIN/DNA)	COMPLEX (DNA-BINDING PROTEIN/DNA) HD; HOMEODOMAIN, COMPLEX	(DNA-BINDING PROTEIN/DNA)	
	Compound		CHAIN: A;	HOMEOBOX VENTRAL NERVOUS SYSTEM DEFECTIVE CHAIN: A;	DNA-BINDING PROTEIN ANTENNAPEDIA PROTEIN (HOMEODOMAIN) MUTANT WITH CYS 39 ISAN 3 REPLACED	BY SER AND RESIDUES 1-6 DELETED (C39S,DEL 1-6) 1SAN 4 (NMR, 20 STRUCTURES) 1SAN 5	DNA-BINDING PROTEIN ANTENNAPEDIA PROTEIN (HOMEODOMAIN) MUTANT WITH CYS 39 1SAN 3 REPLACED BY SER AND RESIDUES 1-6	DELETED (C39S,DEL 1-6) ISAN 4 (NMR, 20 STRUCTURES) ISAN 5	ANTENNAPEDIA PROTEIN; CHAIN: A, B; DNA; CHAIN: C, D,	, я.	ANTENNAPEDIA PROTEIN; CHAIN: A, B; DNA; CHAIN: C, D, E, F;		DNA-BINDING PROTEIN ANTENNAPEDIA PROTEIN
Table 5	SEQ	FOLD					61.49		62.80				
Tal	PMF	score		0.72	1.00						1.00		0.90
	Verify	score		-0.19	-0.24						0.07		0.24
	Psi	Blast		6.8e-17	3.4e-33		3.4e-33		1.7e-32		1.7e-32		5.1e-31
	END	AA		302	302		307		296		296		147
	START	AA		234	242		243		241		241		82
	CHAIN	A		А					А		А		d
	PDB	A		1qry	lsan		lsan		9ant		9ant		1ahd
	SEQ	A Ä		1497	1497	-	1497		1497		1497		1501

	PDB annotation			PROTEIN/DNA	HOMEODOMAIN, DNA, COMPLEX, DNA-BINDING PROTEIN, PROTEIN/DNA	DNA-BINDING PROTEIN ISL-	1HD DNA-BINDING	PROTEIN, HOMEODOMAIN,	LIM DOMAIN	COMPLEX (DNA-BINDING	PROTEIN/DNA) DNA- BINDING PROTEIN DNA	BATTER DOV	FAIKED BOA,	I KANSCKIP I I ON 2	KEGULATION	COMPLEX (DNA-BINDING	PROTEIN/DNA) DNA-	BINDING PROTEIN, DNA,	PAIRED BOX,	TRANSCRIPTION 2	REGULATION	COMPLEX (DNA-BINDING	PROTEIN/DNA) DNA-	BINDING PROTEIN, DNA,	PAIRED BOX,	TRANSCRIPTION 2 REGULATION
	Compound		(HOMEODOMAIN) MUTANT WITH CYS 39 1AHD 3 REPLACED BY SER (C39S) COMPLEX WITH DNA (NMR, 1AHD 4 16 STRUCTURES) 1AHD 5	HOMEOBOX PROTEIN HOX-B1;	CHAIN: A; PBX1; CHAIN: B; DNA CHAIN: D; DNA CHAIN: E;	INSULIN GENE ENHANCER	PROTEIN ISL-1; CHAIN: NULL;			PAIRED PROTEIN; CHAIN: A, B,	C; DNA; CHAIN: D, E, F					PAIRED PROTEIN; CHAIN: A, B,	C; DNA; CHAIN: D, E, F					PAIRED PROTEIN; CHAIN: A, B,	C; DNA; CHAIN: D, E, F			
Table 5	SEQ	FOLD						-								58.65										
Tal	PMF	score		1.00		0.24				1.00												1.00				
	Verify	score		92.0		0.17				0.23												0.18				
	Psi	Blast		1.7e-26		2e-29				1.4e-27						4e-28						4e-28				
	END	AA		142		143				141	٠					145						142				
	START	AA		98		82				81						81						82				
	CHAIN	A		A						Ą						¥						A				
	PDB	A		1672		1bw5				14j1						1fj1 					-	1fj1				
Į	SEÓ	A Ö		1501		1501				1501						1501						1501				

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	PDB annotation	COMPLEX (DNA-BINDING PROTEIN/DNA) DNA- BINDING PROTEIN, DNA, PAIRED BOX, TRANSCRIPTION 2 REGULATION	COMPLEX (DNA-BINDING PROTEIN/DNA) DNA- BINDING PROTEIN, DNA, PAIRED BOX, TRANSCRIPTION 2	COMPLEX (DNA-BINDING PROTEIN/DNA) DNA- BINDING PROTEIN, DNA, PAIRED BOX, TRANSCRIPTION 2 REGULATION		ENDOCYTOSIS/EXOCYTOSI S SYNAPTOTAGMIN ASSOCIATED 35 KDA PROTEIN, P35A, THREE HELIX BUNDLE
	Compound	PAIRED PROTEIN; CHAIN: A, B, C; DNA; CHAIN: D, E, F	PAIRED PROTEIN; CHAIN: A, B, C; DNA; CHAIN: D, E, F	PAIRED PROTEIN; CHAIN: A, B, C; DNA; CHAIN: D, E, F	DNA-BINDING PROTEIN ANTENNAPEDIA PROTEIN (HOMEODOMAIN) MUTANT WITH CYS 39 1SAN 3 REPLACED BY SER AND RESIDUES 1-6 DELETED (C39S,DEL 1-6) 1SAN 4 (NMR, 20 STRUCTURES) 1SAN 5	SYNTAXIN-1A; CHAIN: A, B, C;
Table 5	SEQ FOLD score	55.11				
Tal	PMF score		1.00	1.00	1.00	0.03
	Verify score		0.33	0.33	0.48	-0.27
	Psi Blast	6e-27	3.4e-26	6e-27	1.2e-28	9000
	END AA	138	139	139	147	91
	START AA	82	82	82	88	39
!	CHAIN ID	В	В	В		A
	PDB ID	1fj1	1fj1	1fj1	lsan	1ez3
	SEQ ID NO:	1501	1501	1501	1501	1502

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	PDB annotation			PROTEIN/DNA HOMEODOMAIN, DNA, COMPLEX, DNA-BINDING PROTEIN, PROTEIN/DNA	TRANSCRIPTION/DNA ULTRABITHORAX; PBX PROTEIN; DNA BINDING, HOMEODOMAIN, HOMEOTIC PROTEINS, DEVELOPMENT, 2 SPECIFICTY	DNA BINDING PROTEIN TTF-1 HD; 1FTT 8 DNA BINDING PROTEIN, HOMEODOMAIN, TRANSCRIPTION FACTOR 1FTT 19		COMPLEX (HOMEODOMAIN/DNA) VND/NK-2 HOMEODOMAIN
	Compound		DNA-BINDING PROTEIN ANTENNAPEDIA PROTEIN (HOMEODOMAIN) MUTANT WITH CYS 39 1AHD 3 REPLACED BY SER (C39S) COMPLEX WITH DNA (NMR, 1AHD 4 16 STRUCTURES) 1AHD 5	HOMEOBOX PROTEIN HOX-B1; CHAIN: A; PBX1; CHAIN: B; DNA CHAIN: D; DNA CHAIN: E;	ULTRABITHORAX HOMEOTIC PROTEIN IV; CHAIN: A; HOMEOBOX PROTEIN EXTRADENTICLE; CHAIN: B; DNA (5'- CHAIN: C; DNA (5'- CHAIN: D;	THYROID TRANSCRIPTION FACTOR 1 HOMEODOMAIN; 1FTT 6 CHAIN: NULL; 1FTT 7	DNA-BINDING FUSHI TARAZU PROTEIN (HOMEODOMAIN) (NIMR, 20 STRUCTURES) IFTZ 3	HOMEOBOX PROTEIN VND; CHAIN: P; DNA; CHAIN: A, B;
Table 5	SEQ FOLD	score						
Tal	PMF		0.98	1.00	1.00	66.0	1.00	0.99
	Verify score		0.12	0.33	0.71	99'0	-0.06	0.50
	Psi Blast		1.7e-31	3.4e-26	5.1e-27	3.4e-25	1.2e-26	1.7e-25
	END		08	77	74	82	75	78
	START AA		16	20	20	16	17	6
	CHAIN		d.	A	A			а
	PDB ID		1ahd	1672	1b8i	1# ##	1ftz	1nk2
	SEQ ID	.;	1508	1508	1508	1508	1508	1508

		-1											_								T										
	PDB annotation		VENTRAL NERVOUS	SYSTEM HOMEODOMAIN,	HOMEOBOX, DNA-BINDING	PROTEIN, EMBRYONIC 2	DEVELOPMENT, COMPLEX	(HOMEODOMAIN/DNA)	COMPLEX	(HOMEODOMAIN/DNA)	VND/NK-2 HOMEODOMAIN,	VENTRAL NERVOUS	SYSTEM HOMEODOMAIN,	HOMEOBOX, DNA-BINDING	PROTEIN, EMBRYONIC 2	DEVELOPMENT, COMPLEX	(HOMEODOMAIN/DNA)	HELIX	DNA-BINDING PROTEIN	HELIX-TURN-HELIX, DNA- BINDING PROTEIN								COMPLEX (DNA-BINDING	PROTEIN/DNA) HD;	HOMEODOMAIN, COMPLEX	(DNA-BINDING PROTEIN/DNA)
	Compound								HOMEOBOX PROTEIN VND;	CHAIN: P; DNA; CHAIN: A, B;									HOMEOBOX VENTRAL	NERVOUS SYSTEM DEFECTIVE CHAIN: A;	DNA-BINDING PROTEIN	ANTENNAPEDIA PROTEIN	(HOMEODOMAIN) MUTANT	WITH CYS 39 1SAN 3 REPLACED	BY SER AND RESIDUES 1-6	DELETED (C39S,DEL 1-6) 1SAN 4	(NMR, 20 STRUCTURES) 1SAN 5	ANTENNAPEDIA PROTEIN;	CHAIN: A, B; DNA; CHAIN: C, D,	Б, F;	
Table 5	SEQ FOLD	score																													
Ta	PMF								0.93										0.83		1.00							1.00			
	Verify score								0.43										0.39		0.78							0.39			
	Psi Blast		_						3.4e-24	-									6.8e-25		5.1e-29							3.4e-29			
	END								11										78		80							75			
	START AA		•						15										9		22							20			
	CHAIN								Д.										A									А			
	PDB								1nk3						-				lqry		Isan	•						9ant	•		
	SEQ EQ	SO.							1508										1508		1508		-					1508			

	PDB annotation	OXIDOREDUCTASE FERREDOXIN REDUCTASE; OXIDOREDUCTASE	OXIDOREDUCTASE FERREDOXIN REDUCTASE; OXIDOREDUCTASE	LIPID BINDING PROTEIN GLOBIN FOLD, SIX- STRANDED ANTIPARALLEL BETA SHEET, HELIX- 2 FLANKED FIVE-STRANDED PARALLEL BETA SHEET,	LIPID BINDING 3 PROTEIN	OXIDOREDUCTASE CYTOCHROME P450 REDUCTASE, FNR.	FLAVOPROTEIN, MODULAR 2 PROTEIN,	OXIDOREDUCTASE	FLAVOPROTEIN FERREDOXIN REDUCTASE;	FLAVODOXIN REDUCTASE,	FERREDOXIN REDUCTASE,	OXIDOREDUCTASE,	FLAVOPROTEIN	FLAVOPROTEIN	FERREDOXIN REDUCTASE;	FLAVODOXIN REDUCTASE, FERREDOXIN REDUCTASE,
	Compound	NADPH\.FERREDOXIN OXIDOREDUCTASE; CHAIN: NULL;	NADPHY.FERREDOXIN OXIDOREDUCTASE; CHAIN: NULL;	FLAVOHEMOPROTEIN; CHAIN: A, B		SULFITE REDUCTASE (NADPH) FLAVOPROTEIN ALPHA- CHAIN: A. B:			FLAVODOXIN REDUCTASE; CHAIN: NULL;					FLAVODOXIN REDUCTASE;	CHAIN: NULL;	
Table 5	SEQ FOLD score		98.99						66.92							
Ta	PMF	1.00		86.0		0.13		j						0.84		
	Verify score	0.31		0.29		-0.18								0.44		
	Psi Blast	1.8e-29	1.8e-29	8.5e-41		1.4e-26			1.4e-31					1.4e-31		10.100
	END	306	315	314		309			313					303		
	START AA	70	75	46		98			75					82		
	CHAIN			A		A										
	PDB ID	1a8p	1a8p	lcqx		1ddg			1fdr	A				1fdr		
	SEQ ID NO:	1526	1526	1526		1526			1526					1526		

	PDB annotation		FLAVIN, 2 OXIDOREDUCTASE, FLAVOPROTEIN												OXIDOREDUCTASE	RIBOFLAVIN, FLAVIN	REDUCTASE, FERREDOXIN	KEDUCIASE 2	SUPERFAMILY,	OXIDOREDUCTASE	RIBOFLAVIN, FLAVIN	REDUCTASE, FERREDOXIN	REDUCTASE 2	SUPERFAMILY,	OXIDOREDUCTASE	OXIDOREDUCTASE
	Compound			OXIDOREDUCTASE	(NADP+(A),FERREDOXIN(A)) FERREDOXIN:NADP+	OXIDOREDOCTASE (FERREDOXIN REDITCTASE	1FNB 3 FLAVOENZYME) (E.C.1.18.1.2) 1FNB 4 1FNB 72	ELECTRON TRANSPORT	(FLAVO PROTEIN) CYTOCHROME B=5=	REDUCTASE (E.C.1.6.2.2) 1NDH 3	ELECTRON TRANSPORT	(FLAVO PROTEIN)	CYTOCHROME B=5=	REDUCTASE (E.C.1.6.2.2) INDH 3	FLAVIN REDUCTASE; CHAIN: A,	B, C, D;				FLAVIN REDUCTASE: CHAIN: A.	B, C, D;			-		FLAVIN REDUCTASE; CHAIN: A,
Table 5	SEQ	score		62.28				124.42						!	71.47											
Та	PMF	score									1.00									1.00						0.92
	Verify	score									0.44									0.34				,		0.50
	Psi	Blast		1.6e-21				1.7e-70			1.7e-70				le-33					3.4e-26						1e-33
	END	AA		314				315			315				315					313						303
	START	AA		59				69			70				9/					80						82
,	CHAIN	a a										_			Ą					A	,					А
	PDB	 a		1fnb	**	4.4		1ndh			1ndh	_			1qfj					1afi	2					1qfj
:	SEQ	∃ ÿ		1526				1526			1526				1526					1526						1526

	PDB annotation	RIBOFLAVIN, FLAVIN REDUCTASE, FERREDOXIN REDUCTASE 2 SUPERFAMILY,	OXIDOREDUCTASE OXIDOREDUCTASE FNR; FLAVOENZYME, PHOTOSYNTHESIS, ELECTRON TRANSFER, HYDRIDE 2 TRANSFER,	OXIDOREDUCTASE OXIDOREDUCTASE FNR; FLAVOENZYME, PHOTOSYNTHESIS, ELECTRON TRANSFER, HYDRIDE 2 TRANSFER,	OXIDOREDUCTASE OXIDOREDUCTASE, FLAVOPROTEIN, NADP, FAD, THYLAKOID MEMBRANE, 2 HYCOBILISOME, FNR, NADP+ REDILCTASE	OXIDOREDUCTASE FNR; OXIDOREDUCTASE, FLAVOPROTEIN, NADP, FAD, THYLAKOID MEMBRANE, 2 HYCOBILISOME, FNR, NADP+ REDUCTASE
	Compound	B, C, D;	FERREDOXIN:NADP+ REDUCTASE; CHAIN: A, B;	FERREDOXIN:NADP+ REDUCTASE; CHAIN: A, B;	FERREDOXINNADP+ REDUCTASE; CHAIN: NULL;	FERREDOXINNADP+ REDUCTASE; CHAIN: NULL;
Table 5	SEQ FOLD score		66.01		54.28	
Ta	PMF			0.80		0.47
	Verify score			90.0		0.35
	Psi Blast		2e-29	2e-29	6e-31	6e-31
	END		314	310	313	310
	STAKI		74	72	59	69
	CHAIN		A	A		
444	TUB ID		1qfz	1qfz	1que	1que
Orio	NO.		1526	1526	1526	1526

	PDB annotation									COMPLEX (ZINC	FINGER DINA) COMPLEX (ZINC FINGER DNA), ZINC	FINGER, DNA-BINDING PROTEIN	COMPLEX (ZINC	FINGER/DNA) COMPLEX	(ZINC FINGER/DNA), ZINC	FINGER, DNA-BINDING PROTEIN	TRANSFERASE DINUCLEOTIDE-BINDING
	Compound		OXIDOREDUCTASE (NITROGENOUS ACCEPTOR) NADH-DEPENDENT NITRATE REDUCTASE (CYTOCHROME B	REDUCTASE 2CND 3 FRAGMENT) (E.C.1.6.6.1) COMPLEXED WITH FAD 2CND 4 (SYNCHROTRON X-RAY DIFFRACTION) 2CND 5	OXIDOREDUCTASE (NITROGENOUS ACCEPTOR)	NADH-DEPENDENT NITRATE REDICTASE (CYTOCHROME B	REDUCTASE 2CND 3	FRAGMENT) (E.C.1.6.6.1) COMPLEXED WITH FAD 2CND 4	(SYNCHROTRON X-RAY DIFFRACTION) 2CND 5	QGSR ZINC FINGER PEPTIDE;	CHAIN: A; DUFLEA OLIGONUCLEOTIDE BINDING	SITE; CHAIN: B, C;	QGSR ZINC FINGER PEPTIDE;	CHAIN: A; DUPLEX	OLIGONUCLEOTIDE BINDING	SITE; CHAIN: B, C;	NICOTINATE MONONUCLEOTIDE:5,6- CHAIN:
Table 5	SEQ FOLD	score	111.11														
Tal	PMF score				1.00					0.19			0.57				-0.19
	Verify score				96:0					-0.00			-0.23				0.17
:	Psi Blast		8.5e-68		8.5e-68					1.7e-27			5.1e-28				1.2e-19
	END		315		314					344			373				970
!	START AA		92		78		-			267			290				631
	CHAIN									A			A				A
	PDB ID		2cnd		2cnd	-			•	1a1h			1a1h				1d0s
	SEQ ID	SO:	1526		1526					1532			1532				1532

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	PDB annotation		MOTIF, PHOSPHORIBOSYL TRANSFERASE	COMPLEX (ZINC FINGED	PROTEIN DINA	INTERACTION, PROTEIN	DESIGN, 2 CRYSTAL	STRUCTURE, COMPLEX	(ZINC FINGER/DNA)	COMPLEX (ZINC	FINGER/DNA) ZINC FINGER,	PROTEIN-DNA	INTERACTION, PROTEIN	DESIGN, 2 CRYSTAL	STRUCTURE, COMPLEX	(ZINC FINGER/DNA)	COMPLEX (ZINC	FINGER/DNA) ZINC FINGER,	PROTEIN-DNA	INTERACTION, PROTEIN	DESIGN, 2 CRYSTAL	STRUCTURE, COMPLEX	(ZINC FINGER/DNA)	COMPLEX (TRANSCRIPTION	KEGULATION/DINA)	COMPLEX (TRANSCRIPTION	REGULATION/DNA), RNA	POLYMERASE III, 2	TRANSCRIPTION	INITIATION, ZINC FINGER PROTEIN
	Compound		A;	DNA; CHAIN: A, B, D, E;	PROTEIN: CHAIN: C F G:	inclient, circuit. C, I, C,				DNA; CHAIN: A, B, D, E;	CONSENSUS ZINC FINGER	PROTEIN; CHAIN: C, F, G;					DNA; CHAIN: A, B, D, E;	CONSENSUS ZINC FINGER	PROTEIN; CHAIN: C, F, G;					TFIIIA; CHAIN: A, D; 5S	KIBOSOMAL KINA GEINE; CHAIIN:	B, C, E, F;				
Table 5	SEQ	FOLD									•									-			-							
Taf	PMF	score		0.41						92.0		_					0.00							0.52						
	Verify	score		-0.08						-0.08							0.31							-0.22						
	Psi	Blast		1e-46						6.8e-47							8.5e-10							3.4e-31						
	END	AA	-	342				-		373							432							362						
	START	AA		266						289							402							213						
- 1		CE		ن ن						ပ							G							A						
	PDB	a		1mey	-			., .,,,,		lmey					-		lmey							1tf6						
	SEQ	∃ ÿ		1532						1532							1532							1532						

	PDB annotation	COMPLEX (TRANSCRIPTION REGULATION/DNA) COMPLEX (TRANSCRIPTION REGULATION/DNA), RNA POLYMERASE III, 2 TRANSCRIPTION INITIATION, ZINC FINGER PROTEIN	COMPLEX (TRANSCRIPTION REGULATION/DNA) YING-YANG 1; TRANSCRIPTION INITIATOR ELEMENT, YY1, ZINC 2 FINGER PROTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULATION/DNA)	COMPLEX (TRANSCRIPTION REGULATION/DNA) YING- YANG 1; TRANSCRIPTION INITIATION, INITIATOR ELEMENT, YY1, ZINC 2 FINGER PROTEIN, DNA- PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULATION/DNA)	TRANSCRIPTION REGULATION TRANSCRIPTION REGULATION, ADR1, ZINC FINGER, NMR
	Compound	TFIIIA; CHAIN: A, D; 5S RIBOSOMAL RNA GENE; CHAIN: B, C, E, F;	YYI; CHAIN: C; ADENO- ASSOCIATED VIRUS P5 INITIATOR ELEMENT DNA; CHAIN: A, B;	YY1; CHAIN: C; ADENO- ASSOCIATED VIRUS P5 INITIATOR ELEMENT DNA; CHAIN: A, B;	ADR1; CHAIN: NULL;
Table 5	SEQ FOLD score				
Tal	PMF	0.01	0.52	0.83	-0.17
	Verify score	-0.02	-0.16	0.17	0.01
	Psi Blast	1.7e-33	2.4e-14	1.4e-28	5.1e-08
	END	428	342	373	462
	START	239	241	274	405
	CHAIN	K	U	U	
	PDB ID	1tf6	1ubd	lubd	2adr
	SEQ EQ	1532	1532	1532	1532

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	PDB annotation		LIPID TRANSPORT APO A-I; LIPOPROTEIN, LIPID TRANSPORT,	CHOLESTERÓL METABOLISM, 2 ATHEROSCLEROSIS, HDL, LCAT-ACTIVATION	STRUCTURAL PROTEIN TWO REPEATS OF	SPECTRIN, ALPHA HELICAL LINKER REGION, 2 2	TANDEM 3-HELIX COILED-	COILS, STRUCTURAL PROTEIN	CONTRACTILE PROTEIN	TRIPLE-HELIX COILED	COIL, CONTRACTILE	FROIEIN	COMPLEX (TRANSCRIPTION	REGULATION/DNA)	GABPALPHA; GABPBETA1;	COMPLEX (TRANSCRIPTION	BINDING 2 NIICLEAR	PROTEIN, ETS DOMAIN.	ANKYRIN REPEATS,	TRANSCRIPTION 3 FACTOR	COMPLEX (TRANSCRIPTION REGULATION/DNA)
	Compound		A, B, C, D;		ALPHA SPECTRIN; CHAIN: A, B, C;				HUMAN SKELETAL MUSCLE	ALPHA-ACTININ 2; CHAIN: A;			GA BINDING PROTEIN ALPHA;	CHAIN: A; GA BINDING	PROTEIN BETA 1; CHAIN: B;	DNA; CHAIN: D, E;					GA BINDING PROTEIN ALPHA; CHAIN: A; GA BINDING
Table 5	SEQ FOLD score		26.69		61.27				60.38												
Tal	PMF												-0.15								-0.15
	Verify score												0.02								0.18
	Psi Blast		0.00034		0.00036				7.2e-08				3.4e-29		-						1.7e-30
	END		405		425				416				476								540
	START		210		211				168	,			329								405
	CHAIN		¥.		٧				А				മ								B
	PDB		lavi		1cun		_		1quu ,				lawc								lawc
	SEQ NO:		1533		1533				1533				1534	**				-			1534

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PDB annotation	GABPALPHA, GABPBETA1; COMPLEX (TRANSCRIPTION REGULATION/DNA), DNA- BINDING, 2 NUCLEAR PROTEIN, ETS DOMAIN, ANKYRIN REPEATS, TRANSCRIPTION 3 FACTOR	SIGNAL TRANSDUCTION PROTEIN	SIGNAL TRANSDUCTION PROTEIN	CYTOSKELETON	SIGNALING PROTEIN ARF1 GUANINE NUCLEOTIDE EXCHANGE FACTOR AND PH DOMAIN	PHOSPHOTRANSFERASE RHOGAP DOMAIN; PHOSPHOTRANSFERASE, TPASE ACTIVATING PROTEIN, GAP, CDC42, 2 PHOSPHOINOSITIDE 3- KINASE, SH3 DOMAIN, SH2 DOMAIN, 3 SIGNAL TRANSDUCTION	PHOSPHOTRANSFERASE RHOGAP DOMAIN; PHOSPHOTRANSFERASE, TPASE ACTIVATING PROTEIN, GAP, CDC42, 2
Compound	PROTEIN BETA 1; CHAIN: B; DNA; CHAIN: D, E;	BETA-SPECTRIN; 1BTN 4 CHAIN: NULL; 1BTN 5	BETA-SPECTRIN; 1BTN 4 CHAIN: NULL; 1BTN 5	BETA-SPECTRIN; 1DRO 6 CHAIN: NULL; 1DRO 7	GRP1; CHAIN: A;	PHOSPHATIDYLINOSITOL 3- KINASE; CHAIN: A, B;	PHOSPHATIDYLINOSITOL 3- KINASE; CHAIN: A, B;
SEQ FOLD score							
PMF		0.07	0.99	0.13	0.53	1.00	0.99
Verify score		0.12	0.33	0.19	0.42	0.61	0.46
Psi Blast		4.8e-19	2.4e-07	0.00048	3.6e-13	4.8e-45	1.1e-44
END		809	177	181	177	895	668
START AA		508	06	107	06	720	720
CHAIN					A	∢	В
PDB ID		1btm	1btn	1dro	1fgy	Ipbw	1pbw
SEQ El Si		1534	1534	1534	1534	1534	1534
	PDBCHAINSTARTENDPsiVerifyPMFSEQIDAAAABlastscoreFOLDscorescore	CHAIN START END Psi Verify PMF SEQ Compound ID AA ABlast score score FOLD score Score PROTEIN BETA 1; CHAIN: B; DNA; CHAIN: D, E;	PDB CHAIN START END Psi Verify PMF SEQ Compound ID ID AA AA Blast score score FOLD score Score POLD PROTEIN BETA 1; CHAIN: B; DNA; CHAIN: D, E; Dbm; CHAIN: Dbm;	PDB CHAIN START END Psi Verify PMF SEQ Compound ID AA AA Blast score FOLD score Score PROTEIN BETA 1; CHAIN: B; DNA; CHAIN: B; DNA; CHAIN: D, E; 1bm 508 608 4.8e-19 0.12 0.07 BETA-SPECTRIN; 1BTN 4 CHAIN: 1bm 1bm 90 177 2.4e-07 0.33 0.99 BETA-SPECTRIN; 1BTN 4 CHAIN: 1bm 1bm 90 177 2.4e-07 0.33 0.99 BETA-SPECTRIN; 1BTN 4 CHAIN: 1bm	PDB CHAIN START END Psi Verify Netify PMF SEQ Compound ID ID AA AA Blast score FOLD score Compound ID ID AA Blast score score PROTEIN BETA 1; CHAIN: B; Ib ID A.8e-19 0.12 0.07 BETA-SPECTRIN; IBTN 4 CHAIN: Ibm Ib 90 177 2.4e-07 0.33 0.99 BETA-SPECTRIN; IBTN 4 CHAIN: Ibm Ib 90 177 2.4e-07 0.33 0.99 BETA-SPECTRIN; IBTN 4 CHAIN: Ibm Idro 107 181 0.00048 0.13 0.13 CHAIN: NULL; IBTN 5	PDB CHAIN START END Psi Verify PMF SEQ Compound ID ID AA Blast score score FOLD PROTEIN BETA I; CHAIN: B; Ibin 508 608 4.8e-19 0.12 0.07 BETA-SPECTRIN; IBTN 4 CHAIN: Ibin Ibin 90 177 2.4e-07 0.33 0.99 BETA-SPECTRIN; IBTN 4 CHAIN: Into 6 CHAIN: Into 6 CHAIN: Into 6 CHAIN: NULL; IBTN 5 CHAIN: Into 6 CHAIN: NULL; IDRO 7 CHAIN: NULL; IDRO 7 CHAIN: NULL; IDRO 7 CHAIN: A; Ifgy A 90 177 3.6e-13 0.42 0.53 GRPI; CHAIN: A; Ifgy A 90 177 3.6e-13 0.42 0.53 GRPI; CHAIN: A;	PDB CHAIN START END Psi Verify PMF SEQ Compound ID AA AA Blast score FOLD PROTEIN BETA 1; CHAIN: B; 1bm 508 608 4.8e-19 0.12 0.07 BETA-SPECTRIN; IBTN 4 CHAIN: NULL; IBTN 5 1bm 90 177 2.4e-07 0.33 0.99 BETA-SPECTRIN; IBTN 4 CHAIN: NULL; IBTN 5 1dro 107 181 0.00048 0.19 0.13 BETA-SPECTRIN; IBTN 4 CHAIN: NULL; IBTN 5 1fgy A 90 177 3.6e-13 0.42 0.53 GRD1; CHAIN: NULL; IDRO 6 1fgy A 90 177 3.6e-13 0.42 0.53 GRD1; CHAIN: A; 1pbw A 720 895 4.8e-45 0.61 1.00 PHOSPHATIDYLINOSITOL 3- 1pbw A 720 895 4.8e-45 0.61 1.00 PHOSPHATIDYLIN: A, B;

	PDB annotation	PHOSPHOINOSITIDE 3- KINASE, SH3 DOMAIN, SH2 DOMAIN, 3 SIGNAL TRANSDITCTION	SIGNAL TRANSDUCTION SON OF SEVENLESS; PLECKSTRIN, SON OF SEVENLESS, SIGNAL	SIGNAL TRANSDUCTION SIGNAL TRANSDUCTION SON OF SEVENLESS; PLECKSTRIN, SON OF SEVENLESS, SIGNAL TRANSDUCTION	COMPLEX(GTPASE ACTIVATN/PROTO- ONCOGENE) GTPASE- ACTIVATING PROTEIN RHOGAP; COMPLEX (GTPASE ACTIVATION/PROTO- ONCOGENE), GTPASE, 2 TRANSITION STATE, GAP		TUMOR SUPPRESSOR TUMOR SUPPRESSOR, CDK4/6 INHIBITOR, ANK YRIN MOTTE	COMPLEX (KINASE/ANTI- ONCOGENE) CDK6; P16INK44, MTS1; CYCLIN
	Compound		SOS 1; CHAIN: NULL;	SOS 1; CHAIN: NULL;	P50-RHOGAP; CHAIN: A; TRANSFORMING PROTEIN RHOA; CHAIN: B;	24.00	P19INK4D CDK4/6 INHIBITOR; CHAIN: NULL;	CYCLIN-DEPENDENT KINASE 6; CHAIN: A; MULTIPLE TUMOR SUPPRESSOR; CHAIN: B;
Table 5	SEQ FOLD score							
Ta	PMF	,	0.51	0.39	1.00		-0.19	0.05
	Verify score		0.29	0.10	0.46	004	0.04	0.02
	Psi Blast	,	1.1e-08	2.4e-10	6e-46	2 45 10	5.46-10	3.4e-18
	END		1151	178	668	777	† †	476
	START		1057	88	718	280	707	360
	CHAIN				A			В
F	PDB		1pms	1pms	1tx4	1hd8	2	1bi7
	S E SE		1534	1534	1534	1535		1535

		_					_		_																						
	PDB annotation		DEPENDENT KINASE, CYCLIN DEPENDENT	KINASE INHIBITORY 2	PROTEIN, CDK, INK4, CELL	CYCLE, MULTIPLE TUMOR	SUPPRESSOR, 3 MTS1,	COMPLEX (KINASE/ANTI- ONCOGENE) HEADER	SIGNAL TRANSDUCTION	PROTEIN	SIGNALING PROTEIN	HELIX-TURN-HELIX,	ANKYRIN REPEAT	CYTOSKELETON		SIGNALING PROTEIN ARF1	GUANINE NUCLEOTIDE	EXCHANGE FACTOR AND	PH DOMAIN	SIGNALING PROTEIN ARF1	GUANINE NUCLEOTIDE	EXCHANGE FACTOR AND	PH DOMAIN	CELL CYCLE INHIBITOR	P18-INK4C(INK6); CELL	CYCLE INHIBITOR, P18-	INK4C(INK6), ANKYRIN	REPEAT, 2 CDK 4/6	INHIBITOR	PHOSPHOTRANSFERASE	RHOGAP DOMAIN;
	Compound								BETA-SPECTRIN; 1BTN 4 CHAIN:	NULL; 1BTN 5	CYCLIN-DEPENDENT KINASE 4	INHIBITOR B; CHAIN: A;		BETA-SPECTRIN; 1DRO 6	CHAIN: NULL; 1DRO 7	GRP1; CHAIN: A;				GRP1; CHAIN: A;				CYCLIN-DEPENDENT KINASE 6	INHIBITOR; CHAIN: A, B;					PHOSPHATIDYLINOSITOL 3-	KINASE; CHAIN: A, B;
Table 5	SEQ FOLD	score																													
Ia	PMF score								0.99		-0.13			0.13		0.87				0.53				-0.14						1.00	
	Verify score								0.33		0.21			0.19		0.42				0.42				0.14						0.61	
,	Psi Blast								2.4e-07		le-18			0.00048		4.8e-05				3.6e-13				1.7e-20						4.8e-45	
i.	END								177		481			181		1136				177				445						895	
E	SIAKI AA								06		369			107		1058				3			,,,,	780						720	
T. G. T. T.	CHAIN										V V					₹			-	A			•	¥.						A	
ממת	EUB D								1btn		Idys	******		Idro	,	Itgy				ııgy			1:1.1	quii					 - -	Modi	
OTO	g a S								1535	,	CECI		,	1555		1535			1 7.3 7	C5CI			1676	CCCI					十	csci	

g	SE,	2	CΠJ	7117							2																	
PDB annotation	PHOSPHOTRANSFERASE, TPASE ACTIVATING	PROTEIN, GAP, CDC42,	KINASE SH2 DOMAIN	DOMAIN 3 SIGNAL	TRANSDUCTION	PHOSPHOTRANSFERASE	PHOSPHOTRANSFERASE	TPASE ACTIVATING	PROTEIN, GAP, CDC42, 2	PHOSPHOINOSITIDE 3-	KINASE, SH3 DOMAIN, SH2	DOMAIN, 3 SIGNAL	TRANSDUCTION	SIGNAL TRANSDUCTION	SON OF SEVENLESS;	PLECKSTRIN, SON OF	SEVENLESS, SIGNAL	TRANSDUCTION	SIGNAL TRANSDUCTION	SON OF SEVENLESS;	PLECKSTRIN, SON OF	SEVENLESS, SIGNAL	TRANSDUCTION	COMPLEX(GTPASE	ACTIVATN/PROTO-	ONCOGENE) GTPASE-	ACTIVATING PROTEIN	RHOGAP; COMPLEX
Compound						PHOSPHATIDYLINOSITOL 3-	(1) (1) (1) (1) (1) (1) (1) (1) (1) (1)							SOS 1; CHAIN: NULL;					SOS 1; CHAIN: NULL;					P50-RHOGAP; CHAIN: A;	TRANSFORMING PROTEIN	RHOA; CHAIN: B;		
SEQ FOLD score																												
PMF						0.99							0	0.39					0.39					1.00				
Verify						0.46							,,,	0.16					0.10				,	0.46				
Psi Blast						1.1e-44				_			,	1.2e-06				,	2.4e-10					6e-46				
END AA						668							71,40	1140				0	1/8				000	668				
START AA						720							1057	/01				9	88					/18				
CHAIN					ţ	n											-				_			A				
PDB ID						MgdI							1	1 pms				-	Ipms				7	11X4				
NO EQ					7,07	5551							1525	1227				1676	1333				1575	CSCI				
	PDB CHAIN START END Psi Verify PMF SEQ Compound ID ID AA AA Blast score score FOLD score	PDB CHAIN START END Psi Verify PMF SEQ Compound ID AA AA Blast score FOLD score score FOLD score	PDB CHAIN START END Psi Verify PMF SEQ Compound ID ID AA Blast score score FOLD score	PDB CHAIN START END Psi Verify PMF SEQ Compound ID AA AA Blast score score FOLD score Score sc	PDB CHAIN START END Psi Verify PMF SEQ Compound ID AA AA Blast score score FOLD score scor	PDB CHAIN START END Psi Verify PMF SEQ Compound ID AA AA Blast score FOLD score Scor	PDB CHAIN START END Psi Verify PMF SEQ Compound ID AA AA Blast score score FOLD score Score	PDB CHAIN START END Psi Verify PMF SEQ Compound ID ID AA AA Blast score score FOLD score Score ROLD Score ROLD	PDB CHAIN START END Psi Verify PMF SEQ Compound ID ID AA AA Blast score score FOLD score Ipbw B 720 899 1.1e-44 0.46 0.99 KINASE; CHAIN: A, B;	PDB CHAIN START END Psi Verify PMF SEQ Compound ID AA AA Blast score score FOLD score Ipbw B 720 899 1.1e-44 0.46 0.99	PDB CHAIN START END Psi Verify PMF SEQ Compound ID AA AA Blast score score FOLD score Ipbw B 720 899 1.1e-44 0.46 0.99 RHOSPHATIDYLINOSITOL 3-	PDB CHAIN START END Psi Verify PMF SEQ Compound D AA AA Blast score score FOLD score Ipbw B 720 899 1.1e-44 0.46 0.99 KINASE; CHAIN: A, B;	PDB CHAIN START END Psi Verify PMF SEQ Compound AA AA Blast score score score score score lobund score scor	PDB	PDB CHAIN START END Psi Verify PMF SEQ Compound	PDB	PDB CHAIN START END Psi Verify PMF SEQRE Score Sco	PDB CHAIN START END	PDB CHAIN START END Psi Verify PMF SEQ Compound	PDB CHAIN START END Psi Verify PMF SEQ Compound	PDB CHAIN START END	PDB CHAIN START END Psi Verify PMF SEQ Compound	PDB CHAIN START END Psi Verify PMF SEQ Compound	PDB CHAIN START END Psi Score Score FOLD Score Score FOLD Score Score FOLD Score Score FOLD Score Score Score FOLD Score Score FOLD Score FOLD Score S	PDB CHAIN START END Psi Score Score FOLID Score Score FOLID Score Score FOLID Score Sc	PDB CHAIN START END Psi Verify PMF SEQ Compound	PDB CHAIN START END Psi Verify PMF SEQ Compound	PDB CHAIN START END Psi Score Sc

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	PDB annotation		(GTPASE ACTIVATION/PROTO- ONCOGENE), GTPASE, 2 TRANSITION STATE, GAP	TRANSFERASE TYROSINE- PROTEIN KINASE,	TRANSFERASE, SIGNAL TRANSDUCTION, 2 SH3				COMPLEX (SH3	DOMAIN/VIKAL ENHANCER) SRC-	HOMOLOGY 3 DOMAIN;	COMPLEX (SH3 DOMAIN/VIRAL	ENHANCER), PROTO-	ONCOGENE, 2 TRANSFERASE, TYROSINE-	PROTEIN KINASE,	PHOSPHORYLATION, 3 AIDS, MYRISTYLATION,	GTP-BINDING, ATP-	BINDING, SH3 DOMAIN, 4 SH2 DOMAIN, PPII HELIX,
	Compound			HEMOPOIETIC CELL KINASE; CHAIN: A, B, C, D, E, F;		COMPLEX (ONCOGENE PROTEIN/PEPTIDE) C-CRK (N-	CRKSH3-N) COMPLEXED WITH	ICKA 3 C3G FEF LIDE (FRO-FRO- PRO-ALA-LEU-PRO-PRO-LYS- LYS-ARG) ICKA 4	FYN TYROSINE KINASE; CHAIN:	A, C; HIV-1 NEF PROTEIN; CHAIN: B, D;								
Table 5	SEQ FOI D	score																
Tal	PMF	SCOIC		0.07		0.45			0.40									
	Verify	SCOIE		-0.56		-0.81			-0.15									
	Psi Blast	Didəl		3.4e-11		5.1e-12			8.5e-15									
	END	AA		73		72			71									
	START	¥		30		28			28									
	CHAIN	3		A		A			A									
	PDB	3		1bu1		1cka			1efn									
) () () ()	3 Ġ		536		536			536									

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	PDB annotation	PXXP MOTIF	PHOSPHOTRANSFERASE C- SRC, P60-SRC; SRC, TYROSINF KINASF	PHOSPHORYLATION, SH2, SH3, 2 PHOSPHOTYROSINE, PROTO-ONCOGENE, PHOSPHOTRANSFERASE	TRANSFERASE PROTO- ONCOGENE TYROSINE KINASE; PROTO-	ONCOGENE, TRANSFERASE, TYROSINE-PROTEIN	PHOSPHORYLATION, ATP-	SH3 DOMAIN, 3 COMPLEX	(PHOSPHOTRANSFERASE/PE PTIDE)	COMPLEX	(TRANSFERASE/PEPTIDE) SRC, SH3 DOMAIN	LIGANDS, NON-PEPTIDE	ELEMENTS, 2 COMPLEX	COMPLEX	(TRANSFERASE/PEPTIDE)	JAC, SH3 DOMAIN,	ELEMENTS, 2 COMPLEX	(TRANSFERASE/PEPTIDE)
	Compound		TYROSINE-PROTEIN KINASE SRC; CHAIN: NULL;		PHOSPHOTRANSFERASE FYN; CHAIN: A; 3BP-2; CHAIN: B;					C-SRC; CHAIN: C; NL1 (MN7-	MINZ-MINI-PLPPLP); CHAIN: N;			C-SRC; CHAIN: C; NL1 (MN7-	MN2-MN1-PLPPLP); CHAIN: N;			
Table 5	SEQ FOLD score																	
Ta	PMF		0.34		0.18					-0.19				08.0				
	Verify score		-0.59		-0.20					0.13				-0.33				
	Psi Blast		3.4e-15		1.2e-15					5.1e-09				le-14				
	END		79		73					187				71				
	SIAKI AA		27		27					136				27				
i di Tito	CHAIN				A									S	-			
and	FUB ID		1 fink	· ·	ltyn					Inlo				Inlo				1
000	A C C		1536	,	1536			_		1536				1536				

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	PDB annotation	SIGNAL TRANSDUCTION PROTEIN SRC-HOMOLOGY 3 (SH3) DOMAIN, PEPTIDE- BINDING PROTEIN, 1SEM 18 2 GUANINE NUCLEOTIDE EXCHANGE FACTOR 1SEM		TRANSFERASE HCK; SH3, PROTEIN TYROSINE KINASE, SIGNAL TRANSDUCTION, 2 TRANSFERASE	HYDROLASE TETRATRICOPEPTIDE, TRP; HYDROLASE, PHOSPHATASE, PROTEIN- PROTEIN INTERACTIONS, TPR, 2 SUPER-HELIX, X-RAY STRUCTURE	HYDROLASE TETRATRICOPEPTIDE, TRP; HYDROLASE, PHOSPHATASE, PROTEIN- PROTEIN INTERACTIONS, TPR, 2 SUPER-HELIX, X-RAY STRUCTURE
	Compound	SEM-5; ISEM 3 CHAIN: A, B; ISEM 5 10-RESIDUE PROLINE- RICH PEPTIDE FROM MSOS ISEM 8 CHAIN: C, D ISEM 10	PHOSPHOTRANSFERASE FYN PROTO-ONCOGENE TYROSINE KINASE (E.C.2.7.1.112) 1SHF 3 (SH3 DOMAIN) 1SHF 4	HEMATOPOIETIC CELL KINASE; CHAIN: NULL;	SERINE/THREONINE PROTEIN PHOSPHATASE 5; CHAIN: NULL;	SERINE/THREONINE PROTEIN PHOSPHATASE 5; CHAIN: NULL;
Table 5	SEQ FOLD score					
Tal	PMF	0.43	0.12	60.0	1.00	0.35
	Verify score	-0.64	-0.19	-0.47	-0.11	-0.06
	Psi Blast	1e-12	1.2e-15	3.4e-11	1.5e-22	1.4e-23
	END AA	69	73	73	248	154
	START	31	27	30	134	16
	CHAIN ID	A	A			
	PDB ID	lsem	1shf	4hck	la17	la17
	SEQ NO:	1536	1536	1536	1546	1546

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	PDB annotation		HYDROLASE	TETRATRICOPEPTIDE, TRP;	HYDROLASE,	PHOSPHATASE, PROTEIN-	PROTEIN INTERACTIONS,	TPR, 2 SUPER-HELIX, X-RAY	SIRUCTURE	SIGNALLING COMPLEX	RAC1; P67PHOX;	SIGNALLING COMPLEX,	GTPASE, NADPH OXIDASE,	PROTEIN-PROTEIN 2	COMPLEX, TPR MOTIF	SIGNALLING COMPLEX	RAC1; P67PHOX;	SIGNALLING COMPLEX,	GTPASE, NADPH OXIDASE,	PROTEIN-PROTEIN 2	COMPLEX, TPR MOTIF	CHAPERONE HOP, TPR-	DOMAIN, PEPTIDE-	COMPLEX, HELICAL	REPEAT, HSP90, 2 PROTEIN	BINDING	CHAPERONE HOP, TPR-	DOMAIN, PEPTIDE-	COMPLEX, HELICAL	REPEAT, HSP90, 2 PROTEIN	BINDING	CHAPERONE HOP, TPR-	DOMAIN, PEPTIDE-
	Compound		SERINE/THREONINE PROTEIN	PHOSPHATASE 5; CHAIN: NULL;					7	RAS-RELATED C3 BOTULINUM	TOXIN SUBSTRATE 1; CHAIN: A;	NEUTROPHIL CYTOSOL	FACTOR 2 (NCF-2) CHAIN: B;			RAS-RELATED C3 BOTULINUM	TOXIN SUBSTRATE 1; CHAIN: A;	NEUTROPHIL CYTOSOL	FACTOR 2 (NCF-2) CHAIN: B;			TPR2A-DOMAIN OF HOP;	CHAIN: A; HSP90-PEPTIDE	MEEVD; CHAIN: B;			TPR2A-DOMAIN OF HOP;	CHAIN: A; HSP90-PEPTIDE	MEEVD; CHAIN: B;			TPR2A-DOMAIN OF HOP; CHAN: A: HSD80 DEPTINE	CHAIN. A, HOLYU-FEF 11DE
Table 5	SEQ	FOLD														,							•										
Та	PMF	score	89.0						000	0.89					1,	0.15					,	 90:I					-0.13				!	-0.19	
	Verify	score	0.25						0.15	0.13					000	0.08					;	0.11				000	0.08					0.03	
	Psi	Blast	1.3e-07						2 As 12	5.45-12					2 4 4 4	5.4e-14					0,	0.8e-18	•			,	1.4e-16				;	8.3e-14	
	END	AA	224						240						166	001					0,50	007					140					26	
	START	A.A.	28						101	701					17	7.					177	133				16	10				,	n	
	CHAIN	a				-			В	·					2												ζ		•			ς	
	PDB	3	1a17					-	1e96	· · ·					1006						101					101					10,1		
	SEQ 1	ğ Ş	1546						1546	:					1546						1546					1546					1546		
										-					_		_					_											

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	PDB annotation	COMPLEX, HELICAL REPEAT, HSP90, 2 PROTEIN BINDING	CHAPERONE HOP, TPR- DOMAIN, PEPTIDE- COMPLEX, HELICAL REPEAT, HSP90, 2 PROTEIN BINDING	CHAPERONE HOP, TPR- DOMAIN, PEPTIDE- COMPLEX, HELICAL REPEAT, HSC70, 2 HSP70, PROTEIN BINDING	CHAPERONE HOP, TPR- DOMAIN, PEPTIDE- COMPLEX, HELICAL REPEAT, HSC70, 2 HSP70, PROTEIN BINDING	CHAPERONE HOP, TPR- DOMAIN, PEPTIDE- COMPLEX, HELICAL REPEAT, HSC70, 2 HSP70, PROTEIN BINDING	CHAPERONE HOP, TPR- DOMAIN, PEPTIDE- COMPLEX, HELICAL REPEAT, HSC70, 2 HSP70, PROTEIN BINDING	SIGNALING PROTEIN PEROXISMORE RECEPTOR 1, PTS1-BP, PEROXIN-5, PTS1
	Compound	MEEVD; CHAIN: B;	TPR2A-DOMAIN OF HOP; CHAIN: A; HSP90-PEPTIDE MEEVD; CHAIN: B;	TPR1-DOMAIN OF HOP; CHAIN: A, B; HSC70-PEPTIDE; CHAIN: C, D;	TPR1-DOMAIN OF HOP; CHAIN: A, B; HSC70-PEPTIDE; CHAIN: C, D;	TPR1-DOMAIN OF HOP; CHAIN: A, B; HSC70-PEPTIDE; CHAIN: C, D;	TPR1-DOMAIN OF HOP; CHAIN: A, B; HSC70-PEPTIDE; CHAIN: C, D;	PEROXISOMAL TARGETING SIGNAL 1 RECEPTOR; CHAIN: A, B; PTS1-CONTAINING PEPTIDE;
Table 5	SEQ FOLD score							
Tat	PMF		0.25	1.00	0.17	0.25	0.37	66.0
	Verify	п	0.10	60:00	0.07	0.34	0.02	0.17
	Psi Blast		3.4e-17	3.4e-20	1.5e-17	1.7e-13	2.6e-07	6.8e-31
	END AA		166	249	132	174	194	251
	START		99	132	16	29	96	7
	CHAIN	•	A	⋖	∢	V	Ą	A
	PDB ID		1elr	1elw	lelw	lelw	Ielw	1fch
	SEQ ID NO:		1546	1546	1546	1546	1546	1546

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	PDB annotation	PROTEIN-PEPTIDE COMPLEX, TETRATRICOPEPTIDE REPEAT, TPR, 2 HELICAL REPEAT	PROTEIN TRANSPORT HELIX-TURN-HELIX TPR- LIKE REPEAT, PROTEIN TRANSPORT	PROTEIN TRANSPORT HELIX-TURN-HELIX TPR- LIKE REPEAT, PROTEIN TRANSPORT	PROTEIN TRANSPORT HELIX-TURN-HELIX TPR- LIKE REPEAT, PROTEIN TRANSPORT	KINASE KINASE, SIGNAL TRANSDUCTION, CALCIUM/CALMODULIN	KINASE KINASE, SIGNAL TRANSDUCTION, CALCIUM/CALMODULIN	KINASE KINASE, SIGNAL TRANSDUCTION, CALCIUM/CALMODULIN	KINASE KINASE, SIGNAL TRANSDUCTION, CALCIUM/CALMODULIN	TRANSFERASE
	Compound	CHAIN: C, D;	VESICULAR TRANSPORT PROTEIN SEC17; CHAIN: A;	VESICULAR TRANSPORT PROTEIN SEC17; CHAIN: A;	VESICULAR TRANSPORT PROTEIN SEC17; CHAIN: A;	CALCIUM/CALMODULIN- DEPENDENT PROTEIN KINASE; CHAIN: NULL;	PROTEIN KINASE CK2/ALPHA-			
Table 5	SEQ FOLD score				56.33	72.75	72.75			78.86
Tal	PMF		0.05	0.07				0.82	0.82	
	Verify score		-0.38	0.25				0.02	0.02	
	Psi Blast		5.1e-05	1.4e-10	1.4e-10	3.4e-81	3.4e-81	3.4e-81	3.4e-81	1.5e-42
	END		239	194	253	300	300	286	286	311
	START		109	13	2			9	9	3
	CHAIN		A	A	A					
İ	PDB ID		1qqe	lqqe	1qqe	1a06	1a06	1a06	1a06	1a6o
	SEQ ID NO:		1546	1546	1546	1556	1556	1556	1556	1556

	PDB annotation	TRANSFERASE, SERINE/THREONINE- PROTEIN KINASE, CASEIN KINASE, 2 SER/THR KINASE	TRANSFERASE, TRANSFERASE, SERINE/THREONINE- PROTEIN KINASE, CASEIN KINASE, 2 SER/THR KINASE		
	Compound	SUBUNIT; CHAIN: NULL;	PROTEIN KINASE CK2/ALPHA- SUBUNIT; CHAIN: NULL;	TRANSFERASE(PHOSPHOTRANS FERASE) \$C-/AMP\$-DEPENDENT PROTEIN KINASE (E.C.2.7.1.37) (\$C/APK\$) 1APM 3 (CATALYTIC SUBUNIT) "ALPHA" ISOENZYME MUTANT WITH SER 139 1APM 4 REPLACED BY ALA (/S139A\$) COMPLEX WITH THE PEPTIDE 1APM 5 INHIBITOR PKI(5-24) AND THE DETERGENT MEGA-8 1APM 6	TRANSFERASE(PHOSPHOTRANS FERASE) \$C-/AMP\$-DEPENDENT PROTEIN KINASE (E.C.2.7.1.37) (\$C/APK\$) 1APM 3 (CATALYTIC SUBUNIT) "ALPHA" ISOENZYME MUTANT WITH SER 139 1APM 4 REPLACED BY ALA (/S139A\$) COMPLEX WITH THE PEPTIDE 1APM 5 INHIBITOR PKI(5-24) AND THE DETERGENT MEGA-8 1APM 6
Table 5	SEQ FOLD score		78.86	97.24	97.24
Tal	PMF score				
	Verify				
	Psi Blast		1.5e-42	0	0
	END AA		311	319	319
-	START AA		r.	1	
	CHAIN			កា	ъ
	PDB ID		1a60	lapm	lapm
	SEQ NO.		1556	1556	1556

	PDB annotation			PROTEIN KINASE CDK2; PROTEIN KINASE, CELL CYCLE, PHOSPHORYLATION, STAUROSPORINE, 2 CELL DIVISION, MITOSIS, INHIBITION	PROTEIN KINASE CDK2; PROTEIN KINASE, CELL
	Compound	TRANSFERASE(PHOSPHOTRANS FERASE) \$C-\AMP\$-DEPENDENT PROTEIN KINASE (E.C.2.7.1.37) (\$C/APK\$) 1APM 3 (CATALYTIC SUBUNIT) "ALPHA" ISOENZYME MUTANT WITH SER 139 1APM 4 REPLACED BY ALA (/S139A\$) COMPLEX WITH THE PEPTIDE 1APM 5 INHIBITOR PKI(5-24) AND THE DETERGENT MEGA-8 1APM 6	TRANSFERASE(PHOSPHOTRANS FERASE) \$C-/AMP\$-DEPENDENT PROTEIN KINASE (E.C.2.7.1.37) (\$C/APK\$) 1APM 3 (CATALYTIC SUBUNIT) "ALPHA" ISOENZYME MUTANT WITH SER 139 1APM 4 REPLACED BY ALA (/S139A\$) COMPLEX WITH THE PEPTIDE 1APM 5 INHIBITOR PKI(5-24) AND THE DETERGENT MEGA-8 1APM 6	CYCLIN-DEPENDENT PROTEIN KINASE 2; CHAIN: NULL;	CYCLIN-DEPENDENT PROTEIN KINASE 2; CHAIN: NULL;
Table 5	SEQ FOLD				
Ta	PMF	1.00	1.00	66:0	0.99
	Verify score	0.32	0.32	0.24	0.24
	Psi Blast	0	0	8.5e-56	8.5e-56
	END	284	284	271	271
	START AA	\$	5	5	5
	CHAIN	ш	ш	r.	
	PDB ID	Гарт	lapm	1aq1	laq1
	SEQ P SEQ	1556	1556	1556	1556

	PDB annotation		CYCLE, PHOSPHORYLATION,	STAUROSPORINE, 2 CELL	DIVISION, MITOSIS,	INHIBITION	PROTEIN KINASE CDK2; PROTEIN KINASE, CELI.	CYCLE,	PHOSPHORYLATION,	STAUROSPORINE, 2 CELL	DIVISION, MITOSIS,	INHIBITION	PROTEIN KINASE CDK2;	PROTEIN KINASE, CELL	CYCLE,	FHOSPHOKILAIION,	STAUROSPORINE, 2 CELL	DIVISION, MITOSIS,	COMPLEX	(KINASE/INHIBITOR) CDK6.	P19INK4D; CYCLIN	DEPENDENT KINASE,	CVCLIN DEPENDENT	KINASE INHIBITORY 2	PROTEIN, CDK, INK4, CELL	CYCLE, COMPLEX	(KINASE/INHIBITOR)	HEADER HELIX	COMPLEX (KINASE/INHIBITOR) CDK6;
	Compound						CYCLIN-DEPENDENT PROTEIN. KINASE 2: CHAIN: NIII.I.:						CYCLIN-DEPENDENT PROTEIN	KINASE 2; CHAIN: NULL;					CYCLIN-DEPENDENT KINASE 6:	CHAIN: A C. CVCI IN.	DEPENDENT KINASE	INHIBITOR: CHAIN: B. D;							CYCLIN-DEPENDENT KINASE 6; CHAIN: A, C; CYCLIN-
Table 5	SEQ FOLD	score					81.86						81.86						84.40	:									84.40
Tat	PMF score										,																		
	Verify score																												
	Psi Blast						8.5e-56						8.5e-56						1 4e-45	?	•								1.4e-45
	END AA						314						314						303	1)									303
:	START AA						5						5						9	·									9
	CHAIN			-															A	4									A
	PDB ID						laq1				<u>.</u>		laq1						1hi8	2									1bi8
	SEQ ID	 					1556						1556						1556	227									1556

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	PDB annotation		P19INK4D; CYCLIN	DEPENDENT KINASE,	CYCLIN DEPENDENT	KINASE INHIBITORY 2	PROTEIN, CDK, INK4, CELL	CYCLE, COMPLEX	(KINASE/INHIBITOR)	HEADER HELIX	COMPLEX (INHIBITOR	PROTEIN/KINASE)	INHIBITOR PROTEIN,	CYCLIN-DEPENDENT	KINASE, CELL CYCLE 2	CONTROL, ALPHA/BETA,	COMPLEX (INHIBITOR	PROTEIN/KINASE)	COMPLEX (INHIBITOR	PROTEIN/KINASE)	INHIBITOR PROTEIN,	CYCLIN-DEPENDENT	KINASE, CELL CYCLE 2	CONTROL, ALPHA/BETA,	COMPLEX (INHIBITOR	PROTEIN/KINASE)	TRANSFERASE CSK;	PROTEIN KINASE, C-	TERMINAL SRC KINASE,	PHOSPHORYLATION, 2	STAUROSPORINE,	TRANSFERASE	TRANSFERASE CSK;
	Compound			INHIBITOR; CHAIN: B, D;	<u>ا</u> (X X	<u>a</u>	0	D	\dashv	CYCLIN-DEPENDENT KINASE 6; C	CHAIN: A; P19INK4D; CHAIN: B; P	<u>u</u>	0	K	0	0		CYCLIN-DEPENDENT KINASE 6; C	CHAIN: A; P19INK4D; CHAIN: B; P		0	X X	0	0	P	AL SRC KINASE;	CHAIN: A;		<u>a</u>	<u> </u>		C-TERMINAL SRC KINASE; 1
Table 5	SEQ FOLD	score									19.96			_					19.96		-						74.25						74.25
T	PMF																																
	Verify score																																
	Psi Blast										1e-49								1e-49								1.7e-35						1.7e-35
	END										311								311								278						278
	START AA	•									_								1														1
	CHAIN)				-					A								A								A						A
	PDB ID	}							•		1blx	-							1blx								1byg						1byg
	SEQ	S						,			1556								1556		·				•		1556						1556

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	PDB annotation		PROTEIN KINASE, C- TERMINAL SRC KINASE, PHOSPHORYLATION, 2 STAUROSPORINE, TRANSFERASE							
	Compound		CHAIN: A;	PHOSPHOTRANSFERASE CAMP- DEPENDENT PROTEIN KINASE CATALYTIC SUBUNIT 1CMK 3 (E.C.2.7.1.37) 1CMK 4	PHOSPHOTRANSFERASE CAMP- DEPENDENT PROTEIN KINASE CATALYTIC SUBUNIT 1CMK 3	(E.C.2.7.1.37) 1CMK 4	PHOSPHOTRANSFERASE CAMP- DEPENDENT PROTEIN KINASE CATALYTIC SUBUNIT 1CMK 3 (E.C.2.7.1.37) 1CMK 4	PHOSPHOTRANSFERASE CAMP- DEPENDENT PROTEIN KINASE CATALYTIC SUBUNIT 1CMK 3 (E.C.2.7.1.37) 1CMK 4	TRANSFERASE(PHOSPHOTRANS FERASE) CAMP-DEPENDENT PROTEIN KINASE (E.C.2.7.1.37) (CAPK) 1CTP 3 (CATALYTIC SUBUNIT) 1CTP 4	TRANSFERASE(PHOSPHOTRANS FERASE) CAMP-DEPENDENT PROTEIN KINASE (E.C.2.7.1.37) (CAPK) 1CTP 3 (CATALYTIC SUBUNIT) 1CTP 4
Table 5	SEQ FOI D	score		94.17	94.17				94.73	94.73
Tat	PMF	acore.					1.00	1.00		
	Verify	30036					0.28	0.28		
	Psi Blast	Diasi		0	0		0	0	0	0
ļ	END			319	319		284	284	306	306
	START	¥		-	-		4	4	-	-
	CHAIN			ш	E		тì	ш	EL	Ħ
	PDB	<u> </u>		1cmk	1cmk		1cmk	1cmk	1ctp	1ctp
	SEQ	9 <u>ö</u>		1556	1556		1556	1556	1556	1556

	PDB annotation									TRANSFERASE KINASE	DOMAIN, AUTOINHIBITORY	FRAGINIEM I, HOMODIMEK		TRANSFERASE KINASE	DOMAIN, AUTOINHIBITORY	FRAGMENT, HOMODIMER		PHOSPHOTRANSFERASE	FGFR1K, FIBROBLAST	GROWTH FACTOR	RECEPTOR 1;	TRANSFERASE, TYROSINE-	PROTEIN KINASE, ATP-	BINDING, 2	PHOSPHORYLATION,	RECEPTOR,	PHOSPHOTRANSFERASE	PHOSPHOTRANSFERASE
	Compound		TRANSFERASE(PHOSPHOTRANS FERASE) CAMP-DEPENDENT	PROTEIN KINASE (E.C.2.7.1.37)	(CAPK) 1CTP 3 (CATALYTIC SUBUNIT) 1CTP 4	TRANSFERASE(PHOSPHOTRANS	FERASE) CAMP-DEPENDENT	PROTEIN KINASE (E.C.2./1.3/)	SUBUNIT) 1CTP 4	SERINE/THREONINE-PROTEIN	KINASE PAK-ALPHA; CHAIN: A,	B; SEKINE/ I HKEONINE-	FRO LEIN KINASE FAK-ALFHA; CHAIN: C. D;	SERINE/THREONINE-PROTEIN	KINASE PAK-ALPHA; CHAIN: A,	B; SERINE/THREONINE-	FRO I EIN KINASE FAK-ALFHA; CHAIN: C, D;	FGF RECEPTOR 1; CHAIN: A, B;										FGF RECEPTOR 1; CHAIN: A, B;
Table 5	SEQ	FOLD																86.10										86.10
Ta	PMF	score	1.00			1.00				96.0				86.0														
	Verify	score	0.32			0.32				0.14				0.14														
	Psi	Blast	0			0				5.1e-81				5.1e-81				1.7e-37										1.7e-37
	END	ΑA	292			292				286				286				273										273
	START	AA	4			4				7				7						-								-
	CHAIN	<u> </u>	田			ш				S				S				A										A
	PDB	<u> </u>	1ctp	***		1ctp				1f3m				1f3m				1fgk			-					-		1 fgk
!	SEQ	A Ä	<u> </u>			1556				1556				1556				1556										1556

		T			
	PDB annotation	FGFRIK, FIBROBLAST GROWTH FACTOR RECEPTOR 1; TRANSFERASE, TYROSINE- PROTEIN KINASE, ATP- BINDING, 2 PHOSPHORYLATION, RECEPTOR,	PHOSPHOTRANSFERASE FGRIK, FIBROBLAST GROWTH FACTOR RECEPTOR 1; TRANSFERASE, TYROSINE- PROTEIN KINASE, ATP- BINDING, 2 PHOSPHORYLATION, RECEPTOR,	PHOSPHOTRANSFERASE PHOSPHOTRANSFERASE FGFRIK, FIBROBLAST GROWTH FACTOR RECEPTOR 1; TRANSFERASE, TYROSINE- PROTEIN KINASE, ATP- BINDING, 2 PHOSPHORYLATION, RECEPTOR, PHOSPHORYLATION,	PROTEIN KINASE CDK2; TRANSFERASE,
	Compound		FGF RECEPTOR 1; CHAIN: A, B;	FGF RECEPTOR 1; CHAIN: A, B;	HUMAN CYCLIN-DEPENDENT KINASE 2; CHAIN: NULL;
Table 5	SEQ FOLD score		71.13	71.13	
Ta	PMF				0.99
	Verify score				0.38
	Psi Blast		1.4e-39	1.4e-39	5.1e-59
	END AA		272	272	271
	START				5
	CHAIN		м	В	
	PDB		lfgk	lfgk I	1hc1
010	NO:		1556	1556	1556

			1				т																									
	PDB annotation		SERINE/THREONINE PROTEIN KINASE, ATP-	BINDING, 2 CELL CYCLE,	CELL DIVISION, MITOSIS,	PHOSPHORYLATION	PROTEIN KINASE CDK2;	TRANSFERASE,	SERINE/THREONINE	PROTEIN KINASE, ATP-	BINDING, 2 CELL CYCLE,	CELL DIVISION, MITOSIS,	PHOSPHORYLATION	PROTEIN KINASE CDK2;	TRANSFERASE,	SERINE/THREONINE	PROTEIN KINASE, ATP-	BINDING, 2 CELL CYCLE,	CELL DIVISION, MITOSIS,	PHOSPHORYL ATION	PROTEIN KINASE CDK2;	TRANSFERASE,	SERINE/THREONINE	PROTEIN KINASE, ATP-	BINDING, 2 CELL CYCLE.	CELL DIVISION, MITOSIS	PHOSPHORYLATION	SERINE/THREONINE-	PROTEIN KINASE CSBP, RK,	P38; PROTEIN SER/THR-	KINASE,	SERINE/THREONINE-
	Compound					THE CASE OF STREET	HUMAN CYCLIN-DEPENDENT	MINASE 2; CHAIN: NOLL;						HUMAN CYCLIN-DEPENDENT	KINASE Z; CHAIN: NULL;	,					HUMAN CYCLIN-DEPENDENT	KINASE 2; CHAIN: NULL;						P38 MAP KINASE; CHAIN: NULL;				
Table 5	SEQ FOLD	score											70404	101.86						,0,0	101.86						,	78.76				
Ta	PMF				_	000	66.0																					-				
	Verify score					0.38	00																									
	Psi Blast					5 16-50	V.10-71.0						5 10 50	7.15-77						5 10 50	7.15-73						7 42 42	5.46-42				
í	END AA					271	1 / 2			• •			314	-			_			314							375					
E C	SIAKI AA					5	,				•		\$)			_			2	,							-				
CITATA	CHAIN D																															-
ana	<u>a</u> a					1hcl			-			•	1hcl							1hcl							Tian		_			
CEO) A S					1556							1556							1556							1556					

	PDB annotation	PROTEIN KINASE	SERINE/THREONINE- PROTEIN KINASE CSBP, RK, P38; PROTEIN SER/THR-	KINASE, SERINE/THREONINE- PROTEIN KINASE	COMPLEX (TRANSFERASE/SUBSTRATE) TYROSINE KINASE,	SIGNAL TRANSDUCTION, PHOSPHOTRANSFERASE, 2	COMPLEX (KINASE/PEPTIDE SUBSTRATE/ATP ANALOG),	ENZYME, 3 COMPLEX (TRANSFERASE/SUBSTRATE)	COMPLEX (TRANSFERASE/SUBSTRATE) TYROSINE KINASE.	SIGNAL TRANSDUCTION, PHOSPHOTRANSFERASE, 2	COMPLEX (KINASE/PEPTIDE	SUBSTRATE/ATP ANALOG), ENZYME, 3 COMPLEX	(TRANSFERASE/SUBSTRATE)	TRANSFERASE JNK3; TRANSFERASE, JNK3 MAP	KINASE, SERINE/THREONINE
	Compound		P38 MAP KINASE; CHAIN: NULL;		INSULIN RECEPTOR; CHAIN: A; PEPTIDE SUBSTRATE; CHAIN: B;				INSULIN RECEPTOR; CHAIN: A; PEPTIDE SUBSTRATE; CHAIN: B;					C-JUN N-TERMINAL KINASE; CHAIN: NULL;	
Table 5	SEQ FOLD score		78.76		82.74				82.74	_				89.07	
Ta	PMF														
	Verify score														
	Psi Blast		3.4e-42		1.2e-34				1.2e-34					6.8e-46	
	END		325		289				289					340	
	START AA		_		-									m	
	CHAIN				Ą				∢						
	PDB		lian		1ir3			-	lir3				,	ljnk —	
0 10	NG B SE	,	1556		1556				1556				1	9561	

	PDB annotation	PROTEIN 2 KINASE	TRANSFERASE JNK3; TRANSFERASE JNK3;	KINASE,	SERINE/THREONINE PROTEIN 2 KINA SE	KINASE KINASE, TWITCHIN,	IN I KAS I ERIC REGULATION	KINASE KINASE, TWITCHIN,	KINASE KINASE TWITTER	NTRASTERIC REGIT ATTON	KINASE KINASE, TWITCHIN.	INTRASTERIC REGULATION	KINASE KINASE, TWITCHIN,	INTRASTERIC REGULATION	KINASE KINASE, TWITCHIN,	_		ACTIVATED PROTEIN	KINASE; TRANSFERASE,	MAP KINASE,	SERINE/THREONINE-	PROTEIN KINASE, 2 P38	-		KINASE; TRANSFERASE,	MAP KINASE,	SERINE/THREONINE-	PROTEIN KINASE, 2 P38	KINASE RABBIT MUSCLE
	Compound		C-JUN N-TERMINAL KINASE; CHAIN: NULL;	`		TWITCHIN; CHAIN: NULL;	The same same	TWITCHIN; CHAIN: NULL;	TWITCHIN: CHAIN: A B.	, , , , , , , , , , , , , , , , , , , ,	TWITCHIN; CHAIN: A, B;		TWITCHIN; CHAIN: A, B;		TWITCHIN; CHAIN: A, B;		MAP KINASE P38; CHAIN: NULL;						MAP KINASE P38; CHAIN: NULL;						PHOSPHORYLASE KINASE;
Table 5	SEQ FOLD score	21025	89.07						95.11		95.11						98.98						98.98					70,00	106.76
Ta	PMF					0.99	000	0.99					1.00	,	1.00								,		-				
	Verify score					0.36	200	000					0.13		0.13		•												
	Psi Blast		6.8e-46			6.8e-68	69069	0.05-00	3.4e-67		3.4e-67	,	3.4e-67	1,	3.4e-6/	7	5.1e-48						5.1e-48					\$ 10.70	J.16-/0
	END AA		340			287	787	107	326		326	.,	/97	200	/07	700	175					200	775					090	707
	START		ĸ			5	4)					0	7	-		_						-				-	5	
	CHAIN					-			A		Ą		¥.	<	4							-							
444	PDB ID	,	ljnk			1koa	1koa		1kob	,	lkob	11rot	1KOD	11.0h	0041	128	0001					1220	ocdi	. -			,	1nhk	4
CTC	NO US		1556			1556	1556)	1556	1	1556	1556	0001	1556	200	1556						1556	····					1556	-

	PDB annotation	PHOSPHORYLASE KINASE; GLYCOGEN METABOLISM, TRANSFERASE, SERINE/THREONINE- PROTEIN, 2 KINASE, ATP- BINDING, CALMODULIN- BINDING	KINASE RABBIT MUSCLE PHOSPHORYLASE KINASE; GLYCOGEN METABOLISM, TRANSFERASE, SERINE/THREONINE- PROTEIN, 2 KINASE, ATP- BINDING, CALMODULIN- BINDING	KINASE RABBIT MUSCLE PHOSPHORYLASE KINASE; GLYCOGEN METABOLISM, TRANSFERASE, SERINE/THREONINE- PROTEIN, 2 KINASE, ATP- BINDING, CALMODULIN- BINDING	KINASE RABBIT MUSCLE PHOSPHORYLASE KINASE; GLYCOGEN METABOLISM, TRANSFERASE, SERINE/THREONINE- PROTEIN, 2 KINASE, ATP- BINDING, CALMODULIN- BINDING
	Compound	CHAIN: NULL;	PHOSPHORYLASE KINASE; CHAIN: NULL;	PHOSPHORYLASE KINASE; CHAIN: NULL;	PHOSPHORYLASE KINASE; CHAIN: NULL;
Table 5	SEQ FOLD score		106.76		
La	PMF			1.00	1.00
	Verify score			0.44	0.44
	Psi Blast	-	5.1e-78	5.1e-78	5.1e-78
	END		269	266	266
	STÄRT AA		2	9	6
	CHAIN				
	PDB ID		1 phk	1phk	1plık
) E E E E		1556	1556	1556

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	PDB annotation	TRANSFERASE MAP KINASE, SERINE/THREONINE PROTEIN KINASE,	TRANSFERASE MAP KINASE, SERINE/THREONINE PROTEIN KINASE, TRANSFERASE	SERINE KINASE SERINE KINASE, TITIN, MUSCLE, AUTOINHIBITION	SERINE KINASE SERINE KINASE, TITIN, MUSCLE, AUTOINHIBITION	TRANSFERASE MITOGEN ACTIVATED PROTEIN KINASE, MAP 2, ERK2; TRANSFERASE, SERINE/THREONINE- PROTEIN KINASE, MAP KINASE, 2 ERK2	TRANSFERASE MITOGEN ACTIVATED PROTEIN KINASE, MAP 2, ERK2; TRANSFERASE, SERINE/THREONINE- PROTEIN KINASE, MAP KINASE, 2 ERK2
	Compound	ERK2; CHAIN: NULL;	ERK2; CHAIN: NULL;	TITIN; CHAIN: A, B;	TITIN; CHAIN: A, B;	EXTRACELLULAR REGULÁTED KINASE 2; CHAIN: NULL;	EXTRACELLULAR REGULATED KINASE 2; CHAIN: NULL;
Table 5	SEQ FOLD score	88.01	88.01	91.81	91.81	90.63	90.63
Tal	PMF						
	Verify score						
	Psi Blast	3.4e-44	3.4e-44	3.4e-54	3.4e-54	3.4e-47	3.4e-47
	END	319	319	323	323	324	324
	START AA	П		2	2	1	_
	CHAIN			A	A		
	PDB ID	1pme	1pme	1tki	1tki	3erk	3erk
	SEQ ID NO:	1556	1556	1556	1556	1556	1556

	Γ								\neg	-						_										_								
	PDB annotation			KINASE KINASE, SIGNAL	TRANSDUCTION,	CALCIUM/CALMODULIN	KINASE KINASE, SIGNAL	TRANSDUCTION,	CALCIUM/CALMODULIN	KINASE KINASE, SIGNAL	TRANSDUCTION,	CALCIUM/CALMODULIN	KINASE KINASE, SIGNAL	TRANSDUCTION,	CALCIUM/CALMODULIN	TRANSFERASE	TRANSFERASE,	SERINE/THREONINE-	PROTEIN KINASE, CASEIN	KINASE, 2 SER/THR KINASE	TRANSFERASE	IKANSFEKASE,	SEKINE/THREONINE-	PROTEIN KINASE, CASEIN	KINASE, 2 SER/THR KINASE									
	Compound		The state of the s	CALCIUM/CALMODULIN-	CHAIN: NIII 1:	CAI CHIMICAINGEITHEI	CALCIUM/CALMUDULIN-	DEFENDENT PROTEIN KINASE; CHAIN: NITT I	CALCHUAGOALMONINE	CALCIUM/CALMODULIN-	CHAIN: NITT.	CITAIN: NOLL;	CALCIUM/CALMODULIN-	DEPENDENT PROTEIN KINASE;	CHAIN: NULL;	PROTEIN KINASE CK2/ALPHA-	SUBUNIT; CHAIN; NULL;				PROTEIN KINASE CK2/ALPHA- SUBLINIT: CHAIN: NI II I	coroni, cimini nolli,			ATOTAL STATE	I KANSFEKASE (PHOSPHOTRANS	FEKASE) \$C-/AMP\$-DEPENDENT	PROTEIN KINASE (E.C.2.7.1.37)	(\$C/APK\$) 1APM 3 (CATALYTIC	SUBUNIT) "ALPHA" ISORNZYMF	MUTANT WITH SER 139 1APM 4	REPLACED BY ALA (/S139A\$)	COMPLEX WITH THE PEPTIDE	1APM 5 INHIBITOR PKI(5-24)
Table 5	SEQ	FOLD	score	81.40		81.40	01.10									80.48			_		80.48				104 15	CI.40I								
$\Gamma_{\rm S}$	PMF	score							1	3.1		1	1.00																	**				
	Verify	score							0.15	3		0.15	C1.0														-							
	PSi.	Blast	1 70.83	1.7		1.7e-83	}		1.7e-83	2		1 76-83	7.7.7		.,	0.8e-43				60-47	0.05-43				0	>								
1	END	AA	303)		303			270			270	·		211	311				211	110				319	``								
E	STAKT	¥		ı		1			8			~	,		2	~				3	1		_								-	-	•	
CITABLE	CHAIN	3															-								H		•							
מטמ	20.E	3	1a06			1a06	-		1a06			1a06			1960	000				1afo	2				lapm									
CEO	ਤੂਂ ਵ	N S S	1557			1557			1557	_		1557			1557					1557					1557			-					•	-

-																													
	PDB annotation																												
	Compound		AND THE DETERGENT MEGA-8 1APM 6	TRANSFERASE(PHOSPHOTRANS FERASE) \$C-\AMP\$-DEPENDENT	PROTEIN KINASE (E.C.2.7.1.37)	(\$C/APK\$) 1APM 3 (CATALYTIC	SUBUNIT) "ALFIA" ISUENZYME	MUININ WILLISEN 139 IARIN 4	KEPLACED BY ALA (/SI39A\$)	1 A PM 5 INHIBITOR PK I/5-24)	AND THE DETERGENT MEGA-8	1APM 6	TRANSFERASE(PHOSPHOTRANS	FERASE) \$C-/AMP\$-DEPENDENT	PROTEIN KINASE (E.C.2.7.1.37)	(\$C/APK\$) 1APM 3 (CATALYTIC	SUBUNIT) "ALPHA" ISOENZYME	MUTANT WITH SER 139 1APM 4	REPLACED BY ALA (/S139A\$)	COMPLEX WITH THE PEPTIDE	1APM 5 INHIBITOR PKI(5-24)	AND THE DETERGENT MEGA-8	1APM 6	TRANSFERASE(PHOSPHOTRANS	FERASE) \$C-/AMP\$-DEPENDENT	PROTEIN KINASE (E.C.2.7.1.37)	(\$C/APK\$) 1APM 3 (CATALYTIC	SUBUNIT) "ALPHA" ISOENZYME	MUTANT WITH SER 139 1APM 4 REPLACED BY ALA (/S139A\$)
Table 5	SEQ	FOLD		104.15																									
Tak	PMF	score											1.00											1.00					
	Verify	score											0.54											0.54					
	Psi	Blast		0									0											0					
ļ	END	AA		319							-		265											265					
	START	AA		1									5											5					
	CHAIN	<u> </u>		ப				-					E											田					
	PDB	<u> </u>		lapm	-								lapm					-						1apm					
	SEQ	A Š		1557									1557											1557					

	PDB annotation		PROTEIN KINASE CDK2; PROTEIN KINASE, CELL	PHOSPHORYLATION, STAUROSPORINE, 2 CELL DIVISION, MITOSIS,	PROTEIN KINASE CDK2; PROTEIN KINASE, CELL	CYCLE, PHOSPHORYLATION, STAUROSPORINE, 2 CELL	DIVISION, MITOSIS, INHIBITION	COMPLEX (ISOMERASE/PROTEIN	KINASE) FKBP12; SERINE/THREONINE-	PROTEIN KINASE RECEPTOR R4: COMPI FX	(ISOMERASE/PROTEIN	KINASE), RECEPTOR 2	SERINE/THREONINE KINASE	COMPLEX	(ISOMEKASE/FROTEIN KINASE) FKBP12;
	Compound	COMPLEX WITH THE PEPTIDE 1APM 5 INHIBITOR PKI(5-24) AND THE DETERGENT MEGA-8 1APM 6	CYCLIN-DEPENDENT PROTEIN P. KINASE 2; CHAIN: NULL; P. C.		CYCLIN-DEPENDENT PROTEIN P KINASE 2; CHAIN: NULL;		0		R TYPE	<u>a</u> <u>a</u>	10	. X	S M	ζ;	SUPERFAMILY RECEPTOR TYPE K
Table 5	SEQ FOLD score		88.38		88.38		-	71.44						71.44	
Га	PMF														
	Verify score														
	Psi Blast		1.7e-52		1.7e-52			1.2e-24						1.2e-24	
	END AA		277		277			301				,		301	
	START		5		5			1						1	
	CHAIN ID							В						В	
}	PDB ID		laq1		laq1			1b6c						1b6c	
	SEQ ID NO:		1557		1557			1557						1557	

				r	
	PDB annotation	SERNE/THREONINE- PROTEIN KINASE RECEPTOR R4; COMPLEX (ISOMERASE/PROTEIN KINASE), RECEPTOR 2 SERINE/THREONINE	COMPLEX (KINASE/INHIBITOR) CDK6; P19INK4D; CYCLIN DEPENDENT KINASE, CYCLIN DEPENDENT KINASE INHIBITORY 2 PROTEIN, CDK, INK4, CELL CYCLE, COMPLEX (KINASE/INHIBITOR) HEADER HELIX	COMPLEX (KINASE/INHIBITOR) CDK6; P19INK4D; CYCLIN DEPENDENT KINASE, CYCLIN DEPENDENT KINASE INHIBITORY 2 PROTEIN, CDK, INK4, CELL CYCLE, COMPLEX (KINASE/INHIBITOR) HEADER HELIX	COMPLEX (INHIBITOR PROTEIN/KINASE) INHIBITOR PROTEIN, CYCLIN-DEPENDENT
	Compound	I; CHAIN: B, D, F, H;	CYCLIN-DEPENDENT KINASE 6; CHAIN: A, C; CYCLIN- DEPENDENT KINASE INHIBITOR; CHAIN: B, D;	CYCLIN-DEPENDENT KINASE 6, CHAIN: A, C; CYCLIN- DEPENDENT KINASE INHIBITOR; CHAIN: B, D;	CYCLIN-DEPENDENT KINASE 6; CHAIN: A; P19INK4D; CHAIN: B;
Table 5	SEQ FOLD score		89.80	89.80	102.80
Tal	PMF		*		
	Verify score				
	Psi Blast		5.1e-43	5.1e-43	1.4e-46
	END		303	303	311
	START AA		9	9	
	CHAIN		A	A	A
	PDB ID		16i8	15i8	1blx
	S a S		1557	1557	1557

	PDB annotation	KINASE, CELL CYCLE 2 CONTROL, ALPHA/BETA, COMPLEX (INHIBITOR PROTEIN/KINASE)	COMPLEX (INHIBITOR PROTEIN/KINASE) INHIBITOR PROTEIN, CYCLIN-DEPENDENT KINASE, CELL CYCLE 2 CONTROL, ALPHA/BETA, COMPLEX (INHIBITOR PROTEIN/KINASE)	TRANSFERASE CSK; PROTEIN KINASE, C- TERMINAL SRC KINASE, PHOSPHORYLATION, 2 STAUROSPORINE, TRANSFERASE	TRANSFERASE CSK; PROTEIN KINASE, C- TERMINAL SRC KINASE, PHOSPHORYLATION, 2 STAUROSPORINE, TRANSFERASE		
	Compound		CYCLIN-DEPENDENT KINASE 6; CHAIN: A; P19INK4D; CHAIN: B;	C-TERMINAL SRC KINASE; CHAIN: A;	C-TERMINAL SRC KINASE; CHAIN: A;	PHOSPHOTRANSFERASE CAMP- DEPENDENT PROTEIN KINASE CATALYTIC SUBUNIT 1CMK 3 (E.C.2.7.1.37) 1CMK 4	PHOSPHOTRANSFERASE CAMP- DEPENDENT PROTEIN KINASE CATALYTIC SUBUNIT 1CMK 3
Table 5	SEQ FOLD score		102.80	84.49	84.49	101.22	101.22
Tal	PMF						
	Verify score						
	Psi Blast	!	1.4e-46	3.4e-31	3.4e-31	0	0
	END		311	277	277	319	319
	START AA		-	1	 1	1	
	CHAIN		∀	A	¥	ப	ш
	PDB ID		1blx	1byg	1byg	1 cmk	1cmk
	SEQ B SEQ		1557	1557	1557	1557	1557

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!	PDB annotation					74.																										TRANSFERASE KINASE DOMAIN, AUTOINHIBITORY	
	Compound		(FC27137)1CMK4	PHOSPHOTE ANSFER ASE CAMP.	DEPENDENT PROTEIN KINASE	CATALYTIC SUBUNIT 1CMK 3	(E.C.2.7.1.37) 1CMK 4	PHOSPHOTRANSFERASE CAMP-	DEPENDENT PROTEIN KINASE	CATALYTIC SUBUNIT 1CMK 3	(E.C.2.7.1.37) 1CMK 4	TRANSFERASE(PHOSPHOTRANS	FERASE) CAMP-DEPENDENT	PROTEIN KINASE (E.C.2.7.1.37)	(CAPK) 1CTP 3 (CATALYTIC	SUBUNIT) 1CTP 4	TRANSFERASE(PHOSPHOTRANS	FERASE) CAMP-DEPENDENT	PROTEIN KINASE (E.C.2.7.1.37)	(CAPK) 1CTP 3 (CATALYTIC	SUBUNIT) 1CTP 4	TRANSFERASE(PHOSPHOTRANS	FERASE) CAMP-DEPENDENT	PROTEIN KINASE (E.C.2.7.1.37)	(CAPK) 1CTP 3 (CATALYTIC	SUBUNIT) 1CTP 4	TRANSFERASE(PHOSPHOTRANS	FERASE) CAMP-DEPENDENT	PROTEIN KINASE (E.C.2.7.1.37)	(CAPK) 1CTP 3 (CATALYTIC	SUBUNIT) 1CTP 4	SERINE/THREONINE-PROTEIN KINASE PAK-ALPHA; CHAIN: A,	
Table 5	SEQ	FOLD	3000									103.71					103.71																
Ta	PMF	score		1 00				1.00														1.00					1.00					1.00	
	Verify	score		0.45				0.45														0.34					0.34					-0.09	
	Psi	Blast		0)			0				0					0					0					0					8.5e-56	
	END	AA		265				265				316					316					265			•		265					270	
	START	AA		5	ı			5									_					5					5					7	
	CHAIN	<u>a</u>		H	l			щ				ш					ш					ш					ш					ပ	
	PDB			1cmk				1cmk				1ctp					1ctp					1ctp					1ctp					1f3m	
	SEQ			1557				1557				1557					1557					1557					1557					1557	

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	PDB annotation		FRAGMENT, HOMODIMER	TRANSFERASE KINASE DOMAIN, AUTOINHIBITORY FRAGMENT, HOMODIMER	PHOSPHOTRANSFERASE FGFR1K, FIBROBLAST GROWTH FACTOR RECEPTOR 1; TRANSFERASE, TYROSINE- PROTEIN KINASE, ATP- BINDING, 2 PHOSPHOTRANSFERASE PHOSPHOTRANSFERASE PHOSPHOTRANSFERASE FGFR1K, FIBROBLAST GROWTH FACTOR RECEPTOR 1; TRANSFERASE, TYROSINE- PROTEIN KINASE, ATP- BINDING, 2 PHOSPHORYLATION, RECEPTOR, RECEPTOR 1; TRANSFERASE, TYROSINE- PROTEIN KINASE, ATP- BINDING, 2 PHOSPHORYLATION, RECEPTOR,	PHOSPHOTRANSFERASE FGFR1K, FIBROBLAST GROWTH FACTOR
	Compound		B; SERINE/THREONINE- PROTEIN KINASE PAK-ALPHA; CHAIN: C, D;	SERINE/THREONINE-PROTEIN KINASE PAK-ALPHA; CHAIN: A, B; SERINE/THREONINE- PROTEIN KINASE PAK-ALPHA; CHAIN: C, D;	FGF RECEPTOR 1; CHAIN: A, B; FGF RECEPTOR 1; CHAIN: A, B;	FGF RECEPTOR 1; CHAIN: A, B;
Table 5	SEQ	Score			95.46	79.45
Ta	PMF	score		1.00		
	Verify	score		-0.09		
	Psi	Blast		8.5e-56	1.4e-33 1.4e-33	6.8e-35
	END	AA		270	273	272
	START	AA		7	-1	1
	CHAIN	3		v	A A	В
	PDB	<u> </u>		1f3m	1fgk	1fgk
	SEQ	a ë		1557	1557	1557

	PDB annotation		RECEPTOR 1; TRANSFERASE, TYROSINE-	PROTEIN KINASE, ATP-	BINDING, 2 PHOSPHORYLATION	RECEPTOR,	PHOSPHOTRANSFERASE	PHOSPHOTRANSFERASE FGER 1K FIRRORI AST	GROWTH FACTOR	RECEPTOR 1;	TRANSFERASE, TYROSINE-	BINDING 2	PHOSPHORYLATION,	RECEPTOR,	PHOSPHOTRANSFERASE	PROTEIN KINASE CDK2;	TRANSFERASE,	SERINE/THREONINE	PROTEIN KINASE, ATP-	BINDING, 2 CELL CYCLE,	CELL DIVISION, MITOSIS,	PHOSPHORYLATION	PROTEIN KINASE CDK2;	TRANSFERASE,	SERINE/THREONINE	PROTEIN KINASE, ATP-	BINDING, 2 CELL CYCLE,	CELL DIVISION, MITOSIS,	PHOSPHORYLATION
	Compound							FGF RECEPTOR 1; CHAIN: A, B;								HUMAN CYCLIN-DEPENDENT	KINASE 2; CHAIN: NULL;						HUMAN CYCLIN-DEPENDENT	KINASE 2; CHAIN: NULL;					
Table 5	SEQ FOLD	score						79.45																					
Ta	PMF score															1.00							1.00						
	Verify score															0.56							0.56						
	Psi Blast							6.8e-35								5.1e-55							5.1e-55						
	END							272								269							769						
	START AA							_								5							5						
	CHAIN							a B																					
	PDB				_			lfgk								1hcl	-						lhcl						
	SEQ ID	NO:	··		_			1557								1557							1557				-		

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PDB annotation		PROTEIN KINASE CDK2; TRANSFERASE, SEDINE/THE BONINE	PROTEIN KINASE ATP.	PRINCE SOFT CYCLE	BINDING, 2 CELL CYCLE,	PHOSPHORYLATION	PROTEIN KINASE CDK2;	TRANSFERASE,	SERINE/THREONINE	PROTEIN KINASE, ATP-	BINDING, 2 CELL CYCLE,	CELL DIVISION, MITOSIS,	PHOSPHORYLATION	SERINE/THREONINE-	PROTEIN KINASE CSBP, RK,	P38; PROTEIN SER/THR-	KINASE,	SERINE/THREONINE-	PROTEIN KINASE	SERINE/THREONINE-	PROTEIN KINASE CSBP, RK,	P38; PROTEIN SER/THR-	KINASE,	SERINE/THREONINE-	PROTEIN KINASE	COMPLEX	(TRANSFERASE/SUBSTRATE) TYROSINE KINASE,	SIGNAL TRANSDUCTION,	PHOSPHOTRANSFERASE, 2
Compound		HUMAN CYCLIN-DEPENDENT KINASE 2; CHAIN: NULL;					HUMAN CYCLIN-DEPENDENT	KINASE 2; CHAIN: NULL;			·			P38 MAP KINASE; CHAIN: NULL;						P38 MAP KINASE; CHAIN: NULL;						INSULIN RECEPTOR; CHAIN: A;	PEPTIDE SUBSTRATE; CHAIN: B;			
Table 5 F SEQ	FOLD	107.22					107.22							82.78						82.78						93.03				
PMF	score																													
Verify	score																													
Psi	Blast	5.1e-55					5.1e-55							1.7e-40						1.7e-40						4.8e-30				
END	AA	302					302							325						325						289				
START	AA	5					5							-						,						1				
CHAIN	a																									A				
PDB	<u></u>	Ihcl					1hcl	•						lian						lian			-			1ir3				
SEQ	3 Ö	1557					1557							1557						1557						1557				

	PDB annotation	COMPLEX (KINASE/PEPTIDE SUBSTRATE/ATP ANALOG), ENZYME, 3 COMPLEX (TRANSFERASE/SUBSTRATE)	COMPLEX (TRANSFERASE/SUBSTRATE) TYROSINE KINASE, SIGNAL TRANSDUCTION, PHOSPHOTRANSFERASE, 2 COMPLEX (KINASE/PEPTIDE SUBSTRATE/ATP ANALOG), ENZYME, 3 COMPLEX (TRANSFERASE/SUBSTRATE)	TRANSFERASE JNK3; TRANSFERASE, JNK3 MAP KINASE, SERINE/THREONINE PROTEIN 2 KINASE	TRANSFERASE JNK3; TRANSFERASE, JNK3 MAP KINASE, SERINE/THREONINE PROTEIN 2 KINASE	KINASE KINASE, TWITCHIN, INTRASTERIC REGULATION	KINASE KINASE, TWITCHIN, INTRASTERIC REGULATION	KINASE KINASE, TWITCHIN, INTRASTERIC REGULATION
	Compound		NSULIN RECEPTOR; CHAIN: A; PEPTIDE SUBSTRATE; CHAIN: B;	C-JUN N-TERMINAL KINASE; CHAIN: NULL;	C-JUN N-TERMINAL KINASE; CHAIN: NULL;	TWITCHIN; CHAIN: NULL;	TWITCHIN; CHAIN: NULL;	TWITCHIN; CHAIN: A, B;
Table 5	SEQ FOLD		93.03	91.74	91.74			106.72
Tal	PMF					0.99	66.0	
	Verify score					0.19	0.19	
	Psi Blast		4.8e-30	8.5e-44	8.5e-44	1.7e-68	1.7e-68	8.5e-68
	END		289	341	341	270	270	326
	START			r.	т	5	5	-
	CHAIN		∢					A
	PDB ID		Lir3	1jnk	1 jnk	1koa	1koa	1kob
	SEQ ID		1557	1557	1557	1557	1557	1557

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	PDB annotation		KINASE KINASE, TWITCHIN, INTRASTERIC REGULATION	KINASE KINASE, TWITCHIN,	INTRASTERIC REGULATION	KINASE KINASE, TWITCHIN, INTRASTERIC REGIII. ATION	TRANSFERASE MITOGEN	ACTIVATED PROTEIN	KINASE; TRANSFERASE,	MAP KINASE,	SERINE/THREONINE-	PROTEIN KINASE, 2 P38	TRANSFERASE MITOGEN	ACTIVATED PROTEIN	KINASE; TRANSFERASE,	MAP KINASE,	SERINE/THREONINE-	PROTEIN KINASE, 2 P38	KINASE RABBIT MUSCLE	PHOSPHORYLASE KINASE;	GLYCOGEN METABOLISM,	TRANSFERASE,	SERINE/THREONINE-	PROTEIN, 2 KINASE, ATP-	BINDING, CALMODULIN-	BINDING	KINASE RABBIT MUSCLE	PHOSPHORYLASE KINASE;	GLYCOGEN METABOLISM,	TRANSFERASE, SERINE/THREONINE-
	Compound		TWITCHIN; CHAIN: A, B;	TWITCHIN; CHAIN: A, B;		TWITCHIN; CHAIN: A, B;	MAP KINASE P38; CHAIN: NULL;						MAP KINASE P38; CHAIN: NULL;						PHOSPHORYLASE KINASE;	CHAIN: NULL;							PHOSPHORYLASE KINASE;	CHAIN: NULL;		
Table 5	SEQ FOLD	score	106.72				105.39						105.39						116.22								116.22			
Taf	PMF score			1.00		1.00																								
	Verify score			0.20		0.20																								
	Psi Blast		8.5e-68	8.5e-68		8.5e-68	1.7e-46						1.7e-46						1.7e-80								1.7e-80			
	END		326	268		268	327						327						269								769			
	START AA		-	9		9	l l												5								5			
	CHAIN		А	A		¥			-	-																				
ļ	PDB ID		1kob	1kob		1kob	1p38						1p38				_		1phk								1phk			:
	SEQ	.i NO	1557	1557		1557	1557						1557						1557								1557			

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	PDB annotation	PROTEIN, 2 KINASE, ATP- BINDING, CALMODULIN- BINDING	KINASE RABBIT MUSCLE PHOSPHORYLASE KINASE; GLYCOGEN METABOLISM,	TRANSFERASE, SERINE/THREONINE-	PROTEIN, 2 KINASE, ATP-	BINDING, CALMODULIN- BINDING	KINASE RABBIT MUSCLE PHOSPHORYLASE KINASE;	GLYCOGEN METABOLISM,	TRANSFERASE,	SEKINE/1 HKEONINE-	PROTEIN, 2 KINASE, ATP-	BINDING	TRANSFERASE MAP	SERINE/THREONINE	PROTEIN KINASE,	TRANSFERASE	TRANSFERASE MAP	SERINE/THREONINE	PROTEIN KINASE,	TRANSFERASE	CONTRACTILE PROTEIN TRIPLE-HELIX COILED
	Compound		PHOSPHORYLASE KINASE; CHAIN: NULL;				PHOSPHORYLASE KINASE; CHAIN: NULL;						ERK2; CHAIN: NULL;				ERKZ; CHAIN: NULL;				HUMAN SKELETAL MUSCLE ALPHA-ACTININ 2; CHAIN: A;
Table 5	SEQ FOLD score												97.20				97.20				
Tab	PMF	!	1.00				1.00														0.05
	Verify score		0.50				0.50														0.22
	Psi Blast		1.7e-80				1.7e-80				· ··		6.8e-43				6.8e-43				4.8e-05
	END		269				269						350				350				347
	START		9				9						-				_				239
	CHAIN																				A
	PDB ID		1phk			-	1phk						1pme				1pme				1quu
	SEQ NO.		1557				1557						1557				1557				1557

	PDB annotation		COIL, CONTRACTILE PROTEIN	CONTRACTILE PROTEIN TRIPLE-HELIX COLLED	COIL, CONTRACTILE	PROTEIN	SERINE KINASE SERINE	KINASE, TITIN, MUSCLE,	AUTOINHIBITION	SERINE KINASE SERINE	KINASE, TITIN, MUSCLE,	AUTOINHIBITION	SERINE KINASE SERINE	KINASE, TITIN, MUSCLE,	AUTOINHIBITION	SERINE KINASE SERINE	KINASE, TITIN, MUSCLE,	AUTOINHIBITION	TRANSFERASE MITOGEN	ACTIVATED PROTEIN	KINASE, MAP 2, ERK2;	TRANSFERASE,	SERINE/THREONINE-	PROTEIN KINASE, MAP	KINASE, 2 ERK2	TRANSFERASE MITOGEN	ACTIVATED PROTEIN	KINASE, MAP 2, ERK2;	TRANSFERASE,	SERINE/THREONINE- PROTEIN KINASE MAP	I INC I LILLI I ANALI IL MOLES LILLI DE
	Compound			HUMAN SKELETAL MUSCLE AT PHA-ACTININ 2: CHAIN: A:			TITIN; CHAIN: A, B;			TITIN; CHAIN: A, B;			TITIN; CHAIN: A, B;			TITIN; CHAIN: A, B;			EXTRACELLULAR REGULATED	KINASE 2; CHAIN: NULL;						EXTRACELLULAR REGULATED	KINASE 2; CHAIN: NULL;				
Table 5	SEQ	FOLD					101.04			101.04									100.10							100.10					
Tat	PMF	score		0.05									1.00			1.00															
	Verify	score		0.22		ļ			!				0.33			0.33															
	Psi	Blast		4.8e-05			1e-54			1e-54			1e-54	•		1e-54			3.4e-44							3.4e-44					
	END	AA		347			323			323			266	•		266			348							348					
	START	AA		239			2			2			9			9															
	CHAIN	3		A			A			A			A			A															
	PDB	3		1quu	=		1tki			1tki	•		1tki		-	1tki	-		3erk							3erk					
	SEQ	—— ∋ ÿ		1557			1557			1557			1557			1557			1557							1557					

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	PDB annotation		KINASE, 2 ERK2	P21; SOS; COMPLEX	ONCOGENE	PROTEIN/EXCHANGE	FACTOR), SMALL GTPASE, 2 EXCHANGE FACTOR	P21; SOS; COMPLEX	(ONCOGENE	PROTEIN/EXCHANGE	FACTOR), SMALL GTPASE, 2	EXCHANGE FACTOR	P21; SOS; COMPLEX	ONCOGENE	PROTEIN/EXCHANGE	FACTOR), SMALL GTPASE, 2	EXCHANGE FACTOR	TRANSFERASE BRUTON'S	AGAMMAGLOBULINEMIA	TYROSINE KINASE, BTK;	TRANSFERASE, PH DOMAIN,	BTK MOTIF, ZINC BINDING,	X-LINKED 2	AGAMMAGLOBULINEMIA,	TYROSINE-PROTEIN	KINASE	SIGNAL TRANSDUCTION	PROTEIN	SIGNALING PROTEIN 11	SIGNALING PROTEIN ARF1
	Compound			H-RAS; CHAIN: R; SON OF	SEVENLESS-1; CHAIN: S;			H-RAS; CHAIN: R; SON OF	SEVENLESS-1; CHAIN: S;				H-RAS; CHAIN: R; SON OF	SEVENLESS-1; CHAIN: S;				BRUTON'S TYROSINE KINASE;	CHAIN: A, B;								BETA-SPECTRIN; 1BTN 4 CHAIN:	NULL; IBTN 5	RHO-GEF VAV; CHAIN: A;	GRP1; CHAIN: A;
Table 5	SEQ FOLD	score		196.51																										
Tat	PMF			,	_			1.00					0.05					0.47									0.45		96.0	0.59
	Verify score							90.0					-0.28					0.43									0.53		0.15	0.83
	Psi Blast			2.4e-96				2.4e-96					3.6e-15					6e-05									1.1e-08		2.4e-37	9.6e-16
	END			1549				1548					1001			_		444	·								443		722	447
	START AA			S1153			-	S1209					S946					333									329		548	337
	CHAIN																	А											А	А
	PDB D			1bkd				1bkd					1bkd					1btk	-								1btn		1f5x	1fgy
	SEQ EQ			1563				1563					1563					1563									1563		1563	1563

	PDB annotation	GUANINE NUCLEOTIDE EXCHANGE FACTOR AND PH DOMAIN	SIGNAL TRANSDUCTION SON OF SEVENLESS; PLECKSTRIN, SON OF SEVENLESS, SIGNAL TRANSDUCTION	P21; SOS; COMPLEX (ONCOGENE	PROTEIN/EXCHANGE FACTOR), SMALL GTPASE, 2	EXCHANGE FACTOR	P21; SOS; COMPLEX	ONCOGENE	PROTEIN/EXCHANGE	FACTOR), SMALL GTPASE, 2	EXCHANGE FACTOR	P21; SOS; COMPLEX	(ONCOGENE	PROTEIN/EXCHANGE	FACTOR), SMALL GTPASE, 2	EXCHANGE FACTOR	P21; SOS; COMPLEX	ONCOGENE	PROTEIN/EXCHANGE	\mid FACTOR), SMALL GTPASE, 2	EXCHANGE FACTOR	TRANSFERASE BRUTON'S	AGAIMIMAGEOROPINEMIA
	Compound		SOS 1; CHAIN: NULL;	H-RAS; CHAIN: R; SON OF SEVENLESS-1: CHAIN: S:			H-RAS; CHAIN: R; SON OF	SEVENLESS-1; CHAIN: S;				H-RAS; CHAIN: R; SON OF	SEVENLESS-1; CHAIN: S;				H-RAS; CHAIN: R; SON OF	SEVENLESS-1; CHAIN: S;				BRUTON'S TYROSINE KINASE;	CHAIN: A, B;
Table 5	SEQ FOLD score						197.78														!		
Ta	PMF		-0.15	0.05								1.00					1.00					0.47	
	Verify score		0.19	-0.28								90.0					0.40					0.43	
	Psi Blast		2.4e-12	3.6e-15			2.4e-96					2.4e-96					5.1e-20					6e-05	
	END		445	689	-		1237	_				1236					1235					132	
	START		313	S634			S841					Z897					S994					21	
	CHAIN ID					ļ																A	
	PDB ID		1pms	1bkd			1bkd					15kd					1bkd					1btk	
	SEQ ID NO:		1563	1564			1564					1564					1564					1564	

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	PDB annotation		TYROSINE KINASE, BTK; TRANSFERASE, PH DOMAIN.	BTK MOTIF, ZINC BINDING,	X-LINKED 2	AGAMMAGLOBULINEMIA,	TYROSINE-PROTEIN	KINASE	SIGNAL TRANSDUCTION PROTEIN	SIGNALING PROTEIN 11	ALPHA-HELICES	SIGNALING PROTEIN ARF1	GUANINE NUCLEOTIDE	EXCHANGE FACTOR AND	PH DOMAIN	COMPLEX (BLOOD	COAGULATION/INHIBITOR)	AUTOPROTHROMBIN IIA;	HYDROLASE, SERINE	PROTEINASE), PLASMA	CALCIUM BINDING, 2	GLYCOPROTEIN, COMPLEX	(BLOOD	COAGULATION/INHIBITOR)	GLYCOPROTEIN	MEMBRANE COFACTOR	PROTEIN (MCP); VIRUS	RECEPTOR, COMPLEMENT	COFACTOR, SHORT CONSENSITS REPEAT 2 SCR	מונים בינים בינים בינים מונים
	Compound								BETA-SPECTRIN; 1BTN 4 CHAIN: NULL; 1BTN 5	RHO-GEF VAV; CHAIN: A;		GRP1; CHAIN: A;				ACTIVATED PROTEIN C; CHAIN:	C, L; D-PHE-PRO-MAI; CHAIN: P;								CD46; CHAIN: A, B, C, D, E, F;					
Table 5	SEQ	FOLD											•																	
Tal	PMF	score							0.45	96.0		0.59				-0.17									0.82					
	Verify	score						****	0.53	0.15		0.83				0.14									1.17					
	Psi	Blast							1.1e-08	2.4e-37		9.6e-16				5.1e-11									6e-14					
	END	AA							131	410		135				266									276					
	START	AA							17	236		25				178									220					
	CHAIN	ar								A		A				1								1	A					
	PDB	CII							1btn	1f5x		Ifgy				laut				-					1ckl					
	SEQ	a ö							1564	1564		1564				1570									1570					

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	PDB annotation	MEASLES VIRUS, GLYCOPROTEIN	GLYCOPROTEIN	MEMBRANE COFACTOR	PROTEIN (MCP); VIRUS	RECEPTOR, COMPLEMENT	COFACTOR, SHORT	CONSENSUS REPEAT, 2 SCR,	MEASLES VIRUS,	OLI VOOMBOTERI	MEMBRANE COFACTOR	PROTEIN (MCP): VIRIS	RECEPTOR COMPLEMENT	COFACTOR, SHORT	CONSENSUS REPEAT, 2 SCR,	MEASUES VIRUS	GLYCOPROTEIN	COMPLEMENT INHIBITOR	VCP, SP35; COMPLEMENT,	NMR, MODULES, PROTEIN	STRUCTURE, VACCINIA	VIRUS	COMPLEMENT INHIBITOR	VCP, SP35; COMPLEMENT,	NMR, MODULES, PROTEIN	STRUCTURE, VACCINIA	VIRUS	MATRIX PROTEIN	EXTRACELLULAR MATRIX, CALCIUM-BINDING,
	Compound		CD46; CHAIN: A, B, C, D, E, F;							CRAC CITABLA B C B E E.	CD40, CIIAIIV. A, B, C, D, E, I,							COMPLEMENT CONTROL	PROTEIN; CHAIN: A;				COMPLEMENT CONTROL	PROTEIN; CHAIN: A;				FIBRILLIN; CHAIN: NULL;	
Table 5	SEQ FOLD score				-																								
Tak	PMF		0.00							200	0.01							0.19					-0.15	-				-0.15	
Tal	Verify score		0.53							47.0	40.0							0.58					0.20					0.05	
	Psi Blast	,	2.4e-12	_				-			2.05-1.5							1.2e-11	-				1.2e-13					6.8e-12	
	END		302								201							346					158					289	
	START AA		220					_			40							220					48					216	
ļ	CHAIN		A								¥		-			_		A					A				_		
	PDB ID		1ckl	_							ICKI	**		•				1e5g)				le5g					lemn	
	SEQ ID NO:		1570							0	0/CI							1570					1570					1570	

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	PDB annotation	GLYCOPROTEIN, 2 REPEAT, SIGNAL, MULTIGENE FAMILY, DISEASE	MUTATION, 3 EGF-LIKE	FIBRILLIN-1 FRAGMENT, MATRIX PROTEIN			GLYCOPROTEIN GLYCOPROTEIN	MEMBRANE ADHESION SHORT CONSENSUS	KEFEA1, SUSHI, COMPLEMENT CONTROL PROTEIN 2 N.	TROITIN, Z N- GLYCOSYLATION, MULTI- DOMAIN MEMBRANF	ADHESION	MEMBRANE ADHESION SHORT CONSENSUS	REPEAT, SUSHI, COMPLEMENT CONTROL	PROTEIN, 2 N-GLYCOSYLATION, MULTI-
	Compound				GLYCOPROTEIN 16TH COMPLEMENT CONTROL PROTEIN (/CCP\$) OF FACTOR H 1HCC 3	GLYCOPROTEIN 16TH COMPLEMENT CONTROL PROTEIN (/CCP\$) OF FACTOR H 1HCC 3	LAMININ; CHAIN: NULL;	HUMAN BETA2-GLYCOPROTEIN I; CHAIN: A;				HUMAN BETA2-GLYCOPROTEIN I; CHAIN: A;		
Table 5	SEQ FOLD score											97.15		
Tal	PMF				0.65	0.19	-0.20	-0.18						
	Verify score				0.97	0.22	0.03	0.13						
	Psi Blast				3.6e-14	1.2e-13	1.7e-12	1.4e-14				3.4e-23		
	END				275	104	224	394				361		
	START AA				216	47	51	180				46		ŭ
	CHAIN							V				A		
ļ	PDB ID				1hcc	Thcc	1klo	1qub				1qub		
	SEQ EQ NO:				1570	1570	1570	1570				1570		

	PDB annotation	DOMAIN, MEMBRANE ADHESION	MEMBRANE ADHESION	SHORT CONSENSUS	REPEAT, SUSHI,	COMPLEMENT CONTROL	PROTEIN, 2 N-	GLYCOSYLATION, MULTI-	DOMAIN, MEMBRANE	ADHESION	SPERMADHESIN ACIDIC	SEMINAL PROTEIN;	SPERMADHESIN, BOVINE	SEMINAL PLASMA	PROTEIN, ACIDIC 2	SEMINAL FLUID PROTEIN,	ASFP, CUB DOMAIN, X-RAY	CRYSTAL 3 STRUCTURE,	GROWTH FACTOR	SPERMADHESIN ACIDIC	SEMINAL PROTEIN;	SPERMADHESIN, BOVINE	SEMINAL PLASMA	PROTEIN, ACIDIC 2	SEMINAL FLUID PROTEIN,	ASFP, CUB DOMAIN, X-RAY	CRYSTAL 3 STRUCTURE,	GROWTH FACTOR	COMPLEX (SEMINAL	PLASMA PROTEIN/SPP)	SEMINAL PLASMA
	Compound		HUMAN BETA2-GLYCOPROTEIN	I; CHAIN: A;							ASFP; CHAIN: NULL;									ASFP; CHAIN: NULL;									MAJOR SEMINAL PLASMA	GLYCOPROTEIN PSP-I; CHAIN:	A; MAJOR SEMINAL PLASMA
Table 5	SEQ FOLD score																														
Tal	PMF		-0.03								0.76									0.88					-				0.35		
	Verify		0.08								0.81									0.73									0.89		
	Psi Blast		3.4e-23								6e-27									1.2e-21									4.8e-27		
	END		282								212									394									214		
	START AA		47						_		105						-			272		-							107		
1	CHAIN		A	-																			-						A		
	PDB ID		1qub								1sfp						_			1sfp									lspp	***	
	SEQ ID NO:		1570								1570									1570									1570		

	PDB annotation		PROTEINS,	SPERMADHESINS, CUB	COMPLEY (SEMINAL	COMPLEA (SEMINAL PLASMA PROTEIN/SPP)	COMPLEX (SEMINAL	PLASMA PROTEIN/SPP)	SEMINAL PLASMA	PROTEINS,	SPERMADHESINS, CUB	DOMAIN 2 ARCHITECTURE,	COMPLEX (SEMINAL	PLASMA PROTEIN/SPP)	COMPLEMENT INHIBITOR	SP35, VCP, VACCINIA VIRUS	SP35; COMPLEMENT	INHIBITOR, COMPLEMENT	MODULE, SCR, SUSHI	DOMAIN, 2 MODULE PAIR	COMPLEMENT INHIBITOR	SP35, VCP, VACCINIA VIRUS	SP35; COMPLEMENT	INHIBITOR, COMPLEMENT	MODULE, SCR, SUSHI	DOMAIN, 2 MODULE PAIR	COMPLEMENT INHIBITOR	SP35, VCP, VACCINIA VIRUS	SP35; COMPLEMENT	INHIBITOR, COMPLEMENT	MODULE, SCR, SUSHI	DOMAIN, 2 MODULE PAIR
	Compound		GLYCOPROTEIN PSP-II; CHAIN:	Я			MAJOR SEMINAL PLASMA	GLYCOPROTEIN PSP-I; CHAIN:	A; MAJOR SEMINAL PLASMA	GLYCOPROTEIN PSP-II; CHAIN:	Y				VACCINIA VIRUS	COMPLEMENT CONTROL	PROTEIN; CHAIN; NULL;				VACCINIA VIRUS	COMPLEMENT CONTROL	PROTEIN; CHAIN: NULL;				VACCINIA VIRUS	COMPLEMENT CONTROL	PROTEIN; CHAIN: NULL;			
Table 5	SEQ FOI D	score																														
Ta	PMF	21026					0.94					-			1.00						0.92						90.0		,			
	Verify	21026					0.71								1.00						0.23						-0.02					
	Psi Blast)Carro					3.6e-21								2.4e-16						3.6e-16						5.1e-09		_			
	END						385								305						134						102					
	START	4					279								219						48						7					
	CHAIN	}					A						-					,														
ļ	PDB	}					1spp	·····							lvvc						lvvc						lvvc					
	SEÓ	Ş					1570								1570						1570						1570					

	PDB annotation	GENE REGULATION POZ DOMAIN; PROTEIN- PROTEIN INTERACTION DOMAIN, TRANSCRIPTIONAL 2 REPRESSOR, ZINC-FINGER PROTEIN, X-RAY CRYSTALLOGRAPHY, 3 PROTEIN STRUCTURE, PROMYELOCYTIC LEUKEMIA, GENE REGULATION		TRANSFERASE DINUCLEOTIDE-BINDING MOTIF, PHOSPHORIBOSYL TRANSFERASE	METAL BINDING PROTEIN ZINC-BINDING MODULE, ANKYRIN REPEATS, METAL BINDING PROTEIN	COMPLEX (MOLECULAR CHAPERONE/PEPTIDE) DNAK, HEAT SHOCK PROTEIN 70 KDA (HSP70), COMPLEX 2 (MOLECULAR
	Compound	PROMYELOCYTIC LEUKEMIA ZINC FINGER PROTEIN PLZF; CHAIN: A;	OXIDOREDUCTASE(OXYGEN(A)) GALACTOSE OXIDASE (E.C.1.1.3.9) (PH 4.5) 1GOF 3	NICOTINATE MONONUCLEOTIDE:5,6- CHAIN: A;	PYK2-ASSOCIATED PROTEIN BETA; CHAIN: A;	SUBSTRATE BINDING DOMAIN OF DNAK; CHAIN: A; SUBSTRATE PEPTIDE (7 RESIDUES); CHAIN: B;
Table 5	SEQ FOLD score					
Tal	PMF	09.0	0.10	-0.19	0.72	0.11
	Verify score	0.30	-0.50	0.23	0.12	0.02
	Psi Blast	3.4e-18	1.7e-07	2.4e-12	1.7e-17	0.0024
	END AA	203	466	621	131	310
	START AA	76	411	279	10	228
	CHAIN	V		4	A	A
	PDB ID	1buo	lgof	1d0s	1dcq	1 dkx
	SEQ ID NO:	1571	1571	1572	1577	1577

	PDB annotation	CHAPERONE/PEPTIDE)	CONTRACTILE PROTEIN TRIPLE-HELIX COILED COIL, CONTRACTILE PROTEIN	CONTRACTILE PROTEIN TRIPLE-HELIX COILED COIL, CONTRACTILE PROTEIN	COMPLEX (BLOOD COAGULATION/INHIBITOR) AUTOPROTHROMBIN IIA; HYDROLASE, SERINE PROTEINASE), PLASMA CALCIUM BINDING, 2 GLYCOPROTEIN, COMPLEX (BLOOD COAGULATION/INHIBITOR)	COMPLEX (BLOOD COAGULATION/INHIBITOR) AUTOPROTHROMBIN IIA; HYDROLASE, SERINE PROTEINASE), PLASMA CALCIUM BINDING, 2 GLYCOPROTEIN, COMPLEX (BLOOD COAGULATION/INHIBITOR)	SERINE PROTEINASE COAGULATION FACTOR II;
	Compound		HUMAN SKELETAL MUSCLE ALPHA-ACTININ 2; CHAIN: A;	HUMAN SKELETAL MUSCLE ALPHA-ACTININ 2; CHAIN: A;	ACTIVATED PROTEIN C; CHAIN: C, L; D-PHE-PRO-MAI; CHAIN: P;	ACTIVATED PROTEIN C; CHAIN: C, L; D-PHE-PRO-MAI; CHAIN: P;	THROMBIN LIGHT CHAIN; CHAIN: A, B, C, D; THROMBIN
Table 5	SEQ FOLD score			51.99		51.62	
Tat	PMF	 	0.09		-0.11		-0.18
	Verify score		-0.13		0.22		60.0
	Psi Blast		1.2e-08	1.2e-08	3.6e-10	3.6e-10	1.2e-09
	END		388	340	127	152	151
	START AA		172	94	27	56	31
	CHAIN		А	A	T	J	I
	PDB		1quu	1quu	laut	laut	1dx5
	S B B B B		1579	1579	1582	1582	1582

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	ion		COAGULATION FACTOR II; FETOMODULIN, TM, CD141 ANTIGEN; EGR-CMK SERINE	LIKE	٠		S	SUGAR BINDING PROTEIN	EIN			SUGAR BINDING PROTEIN	EIN			EIN	. •	LLING		EIN	^	LLING		COMPLEX (BLOOD	OR:	TOR,	HEMOPHILIA/EGF, BLOOD	1 102 101 14
	PDB annotation		TON FA JUN, TN SGR-CM	E, EGF-	ULANT	2	VOLYTI	DING P	IN, HEV	DA,	IGEN	DING P	IN, HEV	DA,	CEN	IG PROT	ROTEIN	, SIGNA		IG PROT	ROTEIN	, SIGNA		(BLOOD	S FACT	INHIBI	IA/EGF,	11011, 1
	PDB		AGULAT OMODU TIGEN; I	PROTEINASE, EGF-LIKE	DUMAINS, ANTICOAGULANT	COMPLEX, 2	ANTIFIBRINOLYTIC COMPLEX	AR BIN	UDA; LECTIN, HEVEIN	DOMAIN, UDA	SUPERANTIGEN	AR BIN	UDA; LECTIN, HEVEIN	DOMAIN, UDA,	SUPERANTIGEN	SIGNALLING PROTEIN	BINDING PROTEIN	CYTOKINE, SIGNALLING	PROTEIN	SIGNALLING PROTEIN	BINDING PROTEIN	CYTOKINE, SIGNALLING	PROTEIN	COMPLEX (BLOOD	CHRISTMAS FACTOR;	COMPLEX, INHIBITOR	MOPHIL AGIII AT	2000
			COA FET ANJ	PRC	A Po	<u>S</u>	AN CO	SOC	Z D	<u> </u>	SUP	SOC	<u></u>		SUF	SIG	BIN	CZ	PRC	SIG	BIN	C.Y.	PRC	lo CO		8	HE	3
			HEAVY CHAIN; CHAIN: M, N, O, P; THROMBOMODULIN; CHAIN: I, J, K, L; THROMBIN INHIBITOR	L-GLU-L-GLY-L-ARM; CHAIN: E,				NII	VI/AGGLUTININ ISOLECTIN V;			TIN	VI/AGGLUTININ ISOLECTIN V;			CTOR	, B;			CTOR	, B;			FACTOR IXA; CHAIN: C, L.; D-	, L,			
	Compound	ļ	(; CHAI) (ODUL) (MBIN I	L-ARM				ISOLEC	IN ISOL			ISOLEC	IN ISOL			OSIS F	HAIN: A			OSIS F	HAIN: A			CHAIN:	, CILAII			
	ပိ		Y CHAIN OMBON L; THRC	-L-GLY.	• •			AGGLUTININ ISOLECTIN	SLUTIN	I: A;		AGGLUTININ ISOLECTIN		{: Α;		TUMOR NECROSIS FACTOR	RECEPTOR; CHAIN: A, B;			TUMOR NECROSIS FACTOR	RECEPTOR; CHAIN: A, B;			FACTOR IXA; CHAIN: C, I	JN14-01			
		•	HEAV P; THR I, J, K,	r-GLU	r, c, H;			AGGL	VI/AG	CHAIN: A;		AGGLI	VI/AG	CHAIN: A;		TUMO	RECEP			TUMO	RECEF			FACT(
Table 5	SEQ	FOLD														52.32								52.22				
Ta	PMF	score						0.41				89.0								-0.12								
	Verify	score						0.45				-0.46	-							0.00								
	Psi	Blast						60-99.6				90- 9 9				3.6e-13			:	3.6e-13				8.4e-17				
	END	ΑĄ						105				99				154				143				147				
	START	ΑA	-					26				4				=				4				19				
	CHAIN	<u> </u>						A				A				A				A				L				
	PDB	А	11 11 11					leis				leis				lext				lext				1pfx				
	SEQ	ВŸ						1582				1582				1582				1582				1582				

	PDB annotation	SERINE PROTEASE, CALCIUM-BINDING, HYDROLASE, 3 GLYCOPROTEIN	TRANSFERASE METHYLTRANSFERASE	COMPLEX (TRANSCRIPTION FACTORDNA) COMPLEX (TRANSCRIPTION FACTOR/DNA), TRANSCRIPTION FACTOR, 2 DNA-BINDING PROTEIN	COMPLEX (TRANSCRIPTION FACTOR/DNA) COMPLEX (TRANSCRIPTION FACTOR/DNA), TRANSCRIPTION FACTOR, 2 DNA-BINDING PROTEIN	COMPLEX (TRANSCRIPTION FACTOR/DNA) COMPLEX (TRANSCRIPTION FACTOR/DNA), TRANSCRIPTION FACTOR, 2 DNA-BINDING PROTEIN	OXIDOREDUCTASE FLAVIN- DEPENDENT AMINE OXIDASE,
	Compound		GLYCINE N- METHYLTRANSFERASE; CHAIN: A. B. C. D:	T PROTEIN; CHAIN: A, B, DNA; CHAIN: C, D;	T PROTEIN; CHAÎN: A, B; DNA; CHAÎN: C, D;	T PROTEIN; CHAÎN: A, B; DNA; CHAÎN: C, D;	POLYAMINE OXIDASE; CHAIN: A, B, C;
Table 5	SEQ FOLD score					96.33	
Tal	PMF		0.16	1.00	1.00		0.31
	Verify score		-0.13	-0.11	0.09		-0.01
	Psi Blast	,	3.4e-16	3.4e-51	6e-61	6e-61	8.5e-07
	END		249	143	150	153	98
	START AA		137		1	-	51
	CHAIN		A	<	⋖	∢	A
	PDB ID		1d2h	lxbr	1xbr	1xbr	1637
	SEQ NO 10		1584	1587	1587	1587	1591

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	PDB annotation	OXIDOREDUCTASE	OXIDOREDUCTASE ALPHA- BETA-ALPHA MOTIF.	FLAVIN CONTAINING	OXIDOREDICTASE IRON-	SULFUR FLAVOPROTEIN,	ELECTRON TRANSFER, OXIDOREDITCTASE	COMPLEX	(OXIDOREDUCTASE/TRANS	FERASE) E3BD; REDOX-	ACTIVE CENTER,	GLYCOLYSIS,	OXIDOREDUCTASE	OXIDOREDUCTASE	FLAVOENZYME, OXIDASE,	ENANTIOMERIC	SPECIFICITY, 0-2	AMINOBENZOATE, ACTIVE	SITE FUNNEL, HELICAL	DOMAIN, FAD- 3 BINDING	DOMAIN			.,.				
	Compound		D-AMINO ACID OXIDASE; CHAIN: A:		TRIMETHYI AMINE	DEHYDROGENASE; CHAIN: A,	B;	DIHYDROLIPOAMIDE	DEHYDROGENASE; CHAIN: A,	B; DIHYDROLIPOAMIDE	ACETYLTRANSFERASE; CHAIN:	Ú		L-AMINO ACID OXIDASE;	CHAIN: A, B, C, D, E, F, G, H;							OXIDOREDUCTASE	DIRITIAN OCENTA SET (F. C. 1.8.1.4)	DEH I DROGENASE (E.C.1.8.1.4) COMPI EV WITH 11 PF 3 EI AVIN	COM LEAN WILL DISTANCE	ADENINE-DINUCLEOTIDE (FAD)	OXIDOREDUCTASE (H2O2(A)) NADH PEROXIDASE (NPX)	()
Table 5	SEQ FOLD	acore																									66.44	
Tal	PMF		0.12		0.04			0.05						00.0								0.42						
i	Verify score		-0.57		-0.39			-0.29						-0.46								-0.28						
	Psi Blast		1.7e-05	· ···	1 5e-13			0		-			•	1.2e-10								0					5.1e-59	
	END		262		476			525						150		•						523		-			551	
	START AA		232		37			53			•			49								49					87	
	CHAIN		A		A	4		A						A								A						
	PDB ID		1c0p		1din	; ;		1ebd		-				1f8s								11pf					1nhp	
	SEQ D		1591		1591			1591						1591								1591					1591	

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	PDB annotation			OXIDOREDUCTASE REDOX-ACTIVE CENTER, GLYCOLYSIS, OXIDOREDUCTASE, NAD, 2 FLAVOPROTEIN, FAD, P64K	OXIDOREDUCTASE REDOX- ACTIVE CENTER, GLYCOLYSIS, OXIDOREDUCTASE, NAD, 2 FLAVOPROTEIN, FAD, P64K			OXIDOREDUCTASE NTR; HYPOTHETICAL PROTEIN, REDOX-ACTIVE CENTER, OXIDOREDUCTASE, 2 DISULFIDE
	Compound		(E.C.1.11.1.1) MUTANT WITH CYS 42 INHP 3 REPLACED BY ALA (C42A) INHP 4	SURFACE PROTEIN; CHAIN: NULL;	SURFACE PROTEIN; CHAIN: NULL;	OXIDOREDUCTASE P- HYDROXYBENZOATE HYDROXYLASE (PHBH) (E.C.1.14.13.2) 1PBE 3 COMPLEXED WITH P- HYDROXYBENZOIC ACID 1PBE 4	OXIDOREDUCTASE(FLAVOENZ YME) THIOREDOXIN REDUCTASE (E.C.1.6.4.5) MUTANT WITH CYS 138 1TRB 3 REPLACED BY SER (C138S) 1TRB 4	NADPH DEPENDENT THIOREDOXIN REDUCTASE; CHAIN: NULL;
Table 5	SEQ	FOLD			66.99			
Tal	PMF	score		0.11		0.41	0.51	0.12
	Verify	score		-0.28		-0.25	-0.24	-0.44
	Psi	Blast		3.4e-95	3.4e-95	0.00034	5.16-59	1.7e-53
ļ	END	AA		535	540	08	402	402
	START	AA		45	45	84	,	47
	CHAIN	<u></u>						
	PDB	<u> </u>		lojt	lojt	1pbe	1trb	1vdc
	SEQ	요 일 -		1591	1591	1591	1591	1591

																						-7			
	PDB annotation	OXIDOREDUCTASE, THIOREDOXIN REDUCTASE, FLAVIN 3 ADENINE DINULEOTIDE	OXIDOREDUCTASE SCHAD; OXIDOREDUCTASE, BETA OXIDATION, SCHAD,	CATALYTIC ACTIVITY: 2 L-3-HYDROXYACYL-COA +	+ NADH	OXIDOREDUCTASE SCHAD; OXIDOREDUCTASE, BETA	OXIDATION, SCHAD,	CATALYTIC ACTIVITY: 2 L-	3-HYDROXYACYL-COA+	NAD(+) = 3-0X0ACYL-COA + NADH	OXIDOREDUCTASE SCHAD;	OXIDOREDUCTASE, BETA	OXIDATION, SCHAD,	CATALYTIC ACTIVITY: 2 L-	3-HYDROXYACYL-COA+	NAD(+) = 3-0X0ACYL-COA + NADH	OXIDOREDUCTASE SCHAD;	OXIDOREDUCTASE, BETA	OXIDATION, SCHAD,	CATALYTIC ACTIVITY: 2 L-	3-HYDROXYACYL-COA+	NAD(+) = 3-0X0ACYL-COA			
	Compound		L-3-HYDROXYACYL COA DEHYDROGENASE; CHAIN: A, B, C;			L-3-HYDROXYACYL COA DEHYDROGENASE; CHAIN: A,	B, C;				L-3-HYDROXYACYL COA	DEHYDROGENASE; CHAIN: A,	B, C;				L-3-HYDROXYACYL COA	DEHYDROGENASE; CHAIN: A,	B, C;						
Table 5	SEQ FOLD score																								
Tat	PMF		0.01			0.01			. —		0.00			-			0.25								
	Verify score		-0.11		-0.11											-0.20									
	Psi Blast		0.0014			0.0014					0.0014						0.00014								
	END		84			84					84						98								
	START AA		50		50	50						50													
	CHAIN	<									C						C								
	PDB ID							3hdh						3hdh							3hdh				
	SEQ ID NO:		1591	1591	***				1591						1591										

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	PDB annotation	+ NADH		OXIDOREDUCTASE TRYPANOTHIONE REDUCTASE, FAD DEPENDENT DISULPHIDE 2 OXIDOREDUCTASE	OXIDOREDUCTASE ALPHA-	BETA-ALPHA MOTIF, FLAVIN CONTAINING	PROTEIN, OXIDASE	FLAVOENZYME	FLAVOENZYME, NAD	BIOSYNTHESIS, FAD,	OXIDOREDUCIASE	OXIDOREDUCTASE FLAVOENZYME, OXIDASE,	ENANTIOMERIC	SPECIFICITY, 0-2	AMINOBENZOATE, ACTIVE	SITE FUNNEL, HELICAL	DOMAIN, FAD- 3 BINDING	DOMAIN	OXIDOREDUCTASE FLAVOENZYME, OXIDASE, ENANTIOMERIC	SPECIFICITY, 0-2	
	Compound		OXIDOREDUCTASE DIHYDROLIPOAMIDE DEHYDROGENASE (E.C.1.8.1.4) 3LAD 3	TRYPANOTHIONE REDUCTASE; CHAIN: A, B;	D-AMINO ACID OXIDASE:	CHAIN: A;		L-ASPARTATE OXIDASE;	CHAIN: A;			L-AMINO ACID OXIDASE; CHAIN: A, B, C, D, E, F, G, H;						LO - CLARO CARO - CA LA	L-AMINO ACID OXIDASE; CHAIN: A, B, C, D, E, F, G, H;		
Table 5	SEQ FOLD score																				
Tal	PMF		0.33	0.12	0.17			0.18				00.0							0.23		
	Verify score		-0.36	-0.22	-0.57			0.16				-0.46							-0.13		
	Psi Blast		6.8e- 100	8.5e-76	6.88-05			1.5e-09				1.2e-10							5.1e-09		
	END		523	563	300			414	-			188							135		
	START AA		49	98	070	2		84				87							88		
	CHAIN		A	A	<	:		A				A							4		
	PDB ID		3lad	laog	1002	d	1chu			_	1f8s							1f8s			
	SEQ ID NO:		1591	1592	1500	7661		1592				1592							1592		

	PDB annotation	AMINOBENZOATE, ACTIVE SITE FUNNEL, HELICAL DOMAIN, FAD- 3 BINDING DOMAIN			OXIDOREDUCTASE REDOX- ACTIVE CENTER, GLYCOLYSIS, OXIDOREDUCTASE, NAD, 2 FLAVOPROTEIN, FAD, P64K				
	Compound		OXIDOREDUCTASE DIHYDROLIPOAMIDE DEHYDROGENASE (E.C.1.8.1.4) COMPLEX WITH 1LPF 3 FLAVIN- ADENINE-DINUCLEOTIDE (FAD) 1LPF 4	OXIDOREDUCTASE (H2O2(A)) NADH PEROXIDASE (NPX) (E.C.1.11.1.1) MUTANT WITH CYS 42 INHP 3 REPLACED BY ALA (C42A) INHP 4	SURFACE PROTEIN; CHAIN: NULL;	OXIDOREDUCTASE(FLAVOENZ YME) THIOREDOXIN REDUCTASE (E.C.1.6.4.5) MUTANT WITH CYS 138 1TRB 3 REPLACED BY SER (C138S) 1TRB 4	OXIDOREDUCTASE DIHYDROLIPOAMIDE DEHYDROGENASE (E.C.1.8.1.4) 3LAD 3		
Table 5	SEQ FOLD score			67.46	68.88				
Ta	PMF		0.11			0.30	0.05		
	Verify score		-0.14			-0.09	-0.29		
	Psi Blast		0	1.7e-61	1.5e-96	8.5e-63	3.4e-98		
	END		561	589	578	440	561		
	START		87	125	83	85	87		
	CHAIN		A				A		
	PDB ID		11pf	1nhp	lojt	1trb	3lad		
	SEQ NO.		1592	1592	1592	1592	1592		

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	PDB annotation	LIM DOMAIN CONTAINING PROTEINS LIM DOMAIN CONTAINING PROTEINS, METAL-BINDING PROTEIN, ZINC 2 FINGER	LIM DOMAIN CONTAINING PROTEINS LIM DOMAIN CONTAINING PROTEINS, METAL-BINDING PROTEIN, ZINC 2 FINGER	LIM DOMAIN CONTAINING PROTEINS LIM DOMAIN CONTAINING PROTEINS, METAL-BINDING PROTEIN, ZINC 2 FINGER		PROTEIN/DNA HOMEODOMAIN, DNA, COMPLEX, DNA-BINDING PROTEIN, PROTEIN/DNA	TRANSCRIPTION/DNA ULTRABITHORAX; PBX PROTEIN; DNA BINDING, HOMEODOMAIN, HOMEOTIC PROTEINS,
	Compound	QCRP2 (LIM1); CHAIN: NULL;	QCRP2 (LIM1); CHAIN: NULL;	QCRP2 (LIM1); CHAIN: NULL;	DNA-BINDING PROTEIN ANTENNAPEDIA PROTEIN (HOMEODOMAIN) MUTANT WITH CYS 39 1AHD 3 REPLACED BY SER (C39S) COMPLEX WITH DNA (NMR, 1AHD 4 16 STRUCTURES) 1AHD 5	HOMEOBOX PROTEIN HOX-B1; CHAIN: A; PBX1; CHAIN: B; DNA CHAIN: D; DNA CHAIN: E;	ULTRABITHORAX HOMEOTIC PROTEIN IV; CHAIN: A; HOMEOBOX PROTEIN EXTRADENTICLE; CHAIN: B; DNA (5'- CHAIN: C; DNA (5'-
Table 5	SEQ FOLD score						
Ta	PMF	0.31	0.49	0.75	0.09	0.40	0.71
	Verify score	-0.24	0.14	0.19	-0.25	0.58	0.21
	Psi Blast	1.7e-07	2.2e-18	8.8e-11	1.7e-27	3.4e-24	1e-23
	END AA	98	98	146	256	250	249
	START	25	27	88	191	195	195
	CHAIN				Ь	A	A
	PDB	1a7i	1a7i	1a7i	1ahd	1672	158i
	SEQ ID NO:	1594	1594	1594	1594	1594	1594

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	PDB annotation	DEVELOPMENT, 2 SPECIFICITY	CONTRACTILE LIM	DOMAIN, CRP, NMR,	MUSCLE DIFFERENTIATION,	CONTRACTILE LIM	DOMAIN, CRP, NMR,	MUSCLE DIFFERENTIATION,	CONTRACTILE	CONTRACTILE LIM	DOMAIN, CKP, INMK,	MUSCLE DIFFERENTIATION,	CONTRACTILE	CONTRACTILE LIM	DOMAIN, CRP, NMR,	MUSCLE DIFFERENTIATION,	CONTRACTILE	DNA-BINDING PROTEIN ISL-	1HD DNA-BINDING	PROTEIN, HOMEODOMAIN,	LIM DOMAIN	METAL-BINDING PROTEIN	LIM DOMAIN CONTAINING	PROTEINS 1CTL 15	METAL-BINDING PROTEIN	LIM DOMAIN CONTAINING	PROTEINS 1CTL 15	METAL-BINDING PROTEIN	LIM DOMAIN CONTAINING PROTEINS 1CTL 15	
	Compound	CHAIN: D;	CRP1; CHAIN: A;			CRP1: CHAIN: A:				CRP1; CHAIN: A;				CRP1; CHAIN: A;				INSULIN GENE ENHANCER	PROTEIN ISL-1; CHAIN: NULL;			AVIAN CYSTEINE RICH	PROTEIN; 1CTL 3		AVIAN CYSTEINE RICH	PROTEIN; 1CTL 3		AVIAN CYSTEINE RICH	PROTEIN; 1CTL 3	
Table 5	SEQ FOLD score									55.32								89.50				51.64					. ,			
Tal	PMF		0.04			0.21								0.23											86.0			0.17		
	Verify score		-0.10		-0.19									-0.55											0.09			-0.23		
	Psi Blast		3.4e-10		•	1.7e-11				3.4e-09				3.4e-09				3.4e-17				2e-16			2e-16			1.7e-11		
	END		149			86				279				228	,			254				105			81			86		
	START AA		24			27				85				98				189		,		17			19			27		
	CHAIN ID		A			A				A				A														=	· · · · · ·	
	PDB ID		1b8t	-		1b8t				1b8t		-		1b8t				1bw5	,			1ctl			1ctl			1ctl		
	SEQ ID NO:		1594			1594				1594				1594				1594				1594			1594			1594		

	PDB annotation	METAL-BINDING PROTEIN LIM DOMAIN CONTAINING PROTEINS ICTL 15	METAL-BINDING PROTEIN LIM DOMAIN CONTAINING PROTEINS 1CTL 15	SIGNALING PROTEIN LIM DOMAIN CONTAINING PROTEINS, METAL-BINDING PROTEIN		COMPLEX (DNA-BINDING PROTEIN/DNA) DNA- BINDING PROTEIN, DNA, PAIRED BOX, TRANSCRIPTION 2 REGULATION			
-	Compound	AVIAN CYSTEINE RICH PROTEIN; 1CTL 3	AVIAN CYSTEINE RICH PROTEIN; 1CTL 3	CYSTEINE AND GLYCINE-RICH PROTEIN CRP2; CHAIN: A;	DNA-BINDING PROTEIN ENGRAILED HOMEODOMAIN 1ENH 3	PAIRED PROTEIN; CHAIN: A, B, C; DNA; CHAIN: D, E, F			
Table 5	SEQ FOLD score								
Tat	PMF	0.53	0.34	0.65	0.46	0.99	1.00	0.84	89.0
	Verify score	0.10	-0.13	0.18	0.16	0.53	-0.18	0.21	0.03
	Psi Blast	1.8e-10	5.1e-05	5.1e-09	2e-15	0.0001	1.3e-10	8.5e-18	3.4e-22
	END	143	149	81	83	145	143	245	250
	START AA	88	68	24	27	98	88	193	190
	CHAIN			A	A	A	A		A
	PDB D	1ctl	1ct1	1cxx	1cxx	lcxx	1cxx	1enh	1fj1
	SEQ NO:	1594	1594	1594	1594	1594	1594	1594	1594

	PDB annotation	COMPLEX (DNA-BINDING PROTEIN/DNA) DNA- BINDING PROTEIN, DNA, PAIRED BOX, TRANSCRIPTION 2 REGULATION		METAL-BINDING PROTEIN CRIP; METAL-BINDING PROTEIN, LIM DOMAIN PROTEIN				
	Compound	PAIRED PROTEIN; CHAIN: A, B, C; DNA; CHAIN: D, E, F	DNA-BINDING FUSHI TARAZU PROTEIN (HOMEODOMAIN) (NMR, 20 STRUCTURES) 1FTZ 3	CYSTEINE RICH INTESTINAL PROTEIN; CHAIN: NULL;	DNA-BINDING PROTEIN ANTENNAPEDIA PROTEIN (HOMEODOMAIN) MUTANT WITH CYS 39 ISAN 3 REPLACED BY SER AND RESIDUES 1-6 DELETED (C39S,DEL 1-6) ISAN 4			
Table 5	SEQ FOLD score							
Tal	PMF	0.55	0.12	0.33	09.0	0.42	92.0	0.24
	Verify score	0.08	-0.04	-0.21	-0.13	0.27	0.01	0.27
	Psi Blast	3.4e-21	3.4e-24	1.4e-08	2.2e-21	0.00017	2.2e-10	1.7e-25
	END	248	256	91	66	161	142	256
	START AA	191	190	25	27	87	88	197
	CHAIN	В						
	PDB ID	15)	1ftz	liml	1 iml	1iml	1 iml	1san
	SEQ NO:	1594	1594	1594	1594	1594	1594	1594

	PDB annotation		COMPLEX (DNA BINDING	FRO LEIN/DINA) DINA BINDING, COMPLEX (DNA	BINDING PROTEIN/DNA)	COMPLEX (DNA-BINDING PROTEIN/DNA) HD;	HOMEODOMAIN, COMPLEX	(DNA-BINDING PROTEIN/DNA)		COMPLEX (INHIBITOR/NUCLEASE)	COMPLEX	(INHIBITOR/NUCLEASE),	COMPLEX (KI-ANG), HYDBOI ASE 2 MOI ECTIT AB	DECOCNITION EDITODE	MAPPING LELICINE-RICH 3	REPEATS	COMPLEX	(INHIBITOR/NUCLEASE)	COMPLEX	(INHIBITOR/NUCLEASE),	COMPLEX (RI-ANG),	HYDROLASE 2 MOLECULAR	RECOGNITION, EPITOPE	MAPPING, LEUCINE-RICH 3	REPEATS	COMPLEX (INHIBITOR/NUCLEASE)
	Compound	(NMR 20 STRUCTURES) ISAN 5	ENGRAILED HOMEODOMAIN;	CHAIN: C, D;		ANTENNAPEDIA PROTEIN; CHAIN: A, B; DNA; CHAIN: C, D,	Б, F;			RIBONUCLEASE INHIBITOR; CHAIN: A, D; ANGIOGENIN;	CHAIN: B, E;						RIBONUCLEASE INHIBITOR;	CHAIN: A, D; ANGIOGENIN;	CHAIN: B, E;							RIBONUCLEASE INHIBITOR; CHAIN: A, D; ANGIOGENIN;
Table 5	SEQ FOLD	SCOIC																								
Ta	PMF		0.72			0.34				0.94							1.00									1.00
	Verify score		0.34			0.19				0.30							0.28									0.32
	Psi Blast		1.2e-17			1.4e-25				3.4e-32							1.2e-48									3.6e-23
	END AA		247			250				354			,				414	•								330
	START AA		192		1	195				158			11				168								1	37
	CHAIN		В			V				А		-					A									A
	PDB ID		2hdd			9ant			,	la4y						,	la4y									1a4y
) H S H S		1594		, 0,	1594				1791				,		,	1791									1621

	PDB annotation	COMPLEX (INHIBITOR/NUCLEASE), COMPLEX (RI-ANG), HYDROLASE 2 MOLECULAR RECOGNITION, EPITOPE MAPPING, LEUCINE-RICH 3 REPEATS	COMPLEX (INHIBITOR/NUCLEASE) COMPLEX (INHIBITOR/NUCLEASE), COMPLEX (RI-ANG), HYDROLASE 2 MOLECULAR RECOGNITION, EPITOPE MAPPING, LEUCINE-RICH 3 REPEATS	CELL ADHESION LEUCINE RICH REPEAT, CALCIUM BINDING, CELL ADHESION	TRANSFERASE CRYSTAL STRUCTURE, RAB GERANYLGERANYLTRANSF ERASE, 2.0 A 2 RESOLUTION, N- FORMYLMETHIONINE, ALPHA SUBUNIT, BETA SUBUNIT	RNA BINDING PROTEIN TAP (NFX1); RIBONUCLEOPROTEIN (RNP,RBD OR RRM) AND
	Compound	CHAIN: B, E;	RIBONUCLEASE INHIBITOR; CHAIN: A, D; ANGIOGENIN; CHAIN: B, E;	INTERNALIN B; CHAIN: A;	RAB GERANYLGERANYLTRANSFER ASE ALPHA SUBUNIT; CHAIN: A, C; RAB GERANYLGERANYLTRANSFER ASE BETA SUBUNIT; CHAIN: B, D;	NUCLEAR RNA EXPORT FACTOR 1; CHAIN: A, B;
Table 5	SEQ FOLD score					
Tal	PMF		1.00	0.28	0.06	60.0
	Verify		0.44	0.13	0.02	0.46
	Psi Blast		6e-19	8.5e-07	8.5e-05	5.1e-05
	END AA		427	398	278	303
	START AA		40	237	170	168
	CHAIN		Ą	A	Ą	В
	PDB ID		1a4y	140b	1dce	1fo1
	SEQ ID NO:	nadar Podr Abbrida na to	1621	1621	1621	1621

		T																								
	PDB annotation	LEUCINE-RICH-REPEAT 2 (LRR)	LIGASE CYCLIN A/CDK2- ASSOCIATED PROTEIN P45;	CYCLIN A/CDK2-	ASSOCIATED PROTEIN P19; SKP1. SKP2. F-BOX. LRR	LEUCINE-RICH REPEAT,	SCF, UBIQUITIN, 2 E3,	USIQUITIN PROTEIN LIGASE	LIGASE CYCLIN A/CDK2- ASSOCIATED PROTEIN P45:	CYCLIN A/CDK2-	ASSOCIATED PROTEIN P19;	SKP1, SKP2, F-BOX, LRR,	LEUCINE-RICH REPEAT,	SCF, UBIQUITIN, 2 E3,	UBIQUITIN PROTEIN LIGASE	TRANSCRIPTION RNA1P;	RANGAP; GTPASE-	ACTIVATING PROTEIN FOR	SPI1, GTPASE-ACTIVATING	PROTEIN, GAP, RNA1P,	RANGAP, LRR, LEUCINE- 2	RICH REPEAT PROTEIN,	TWINNING, HEMIHEDRAL	TWINNING, 3 MEROHEDRAL	TWINNING, MEROHEDRY	ACETYLATION RNASE
	Compound		SKP2; CHAIN: A, C, E, G, I, K, M, O; SKP1; CHAIN: B, D, F, H, J, L,	Z, P;					SKP2; CHAIN: A, C, E, G, I, K, M, O; SKP1; CHAIN: B, D, F, H, J, L,	N, P;						GTPASE-ACTIVATING PROTEIN	RNA1_SCHPO; CHAIN: A, B;									RIBONUCLEASE INHIBITOR;
Table 5	SEQ FOLD score																									
Ia	PMF		0.63						06.0							0.35									0	0.98
	Verify score		0.46						0.20							0.38										0.15
	Fsi Blast		9600.0						9.6e-07							1.5e-12				•					7 7	1./e-52
9	AA		110						788							408	17				•				414	414
CTADT	AA		36						0				•	·	į	/51									160	100
CUADA	CILAIN		A					-	€							¥		•								
ana			liqv	-				15.	, bir							1)1g									2hnh	4.DIMI
CEO	NO IO	.0,	1791					1601	1021						1631	1071									1691	1021

	PDB annotation	INHIBITOR, RIBONUCLEASE/ANGIOGEN IN INHIBITOR	ACETYLATION, LEUCINE- RICH REPEATS	ACETYLATION RNASE INHIBITOR,	RIBONUCLEASE/ANGIOGEN IN INHIBITOR	ACETYLATION, LEUCINE- RICH REPEATS	ACETYLATION RNASE	RIBONUCLEASE/ANGIOGEN	IN INHIBITOR	ACETYLATION, LEUCINE- RICH REPEATS	TOXIN BINDING PROTEIN	TWO DOMAINS: BETA	PROPELLER AND ALPHA/BETA FOLD	TOXIN BINDING PROTEIN	TWO DOMAINS: BETA	PROPELLER AND	ALPHA/BETA FOLD	TOXIN BINDING PROTEIN	TWO DOMAINS: BETA	PROPELLER AND	ALPHA/BETA FOLD	I UALIN DILADILAU F NU LELIN
	Compound	CHAIN: NULL;		RIBONUCLEASE INHIBITOR; CHAIN: NULL;			RIBONUCLEASE INHIBITOR; CHAIN: NI II I				TOLB PROTEIN; CHAIN: A;			TOLB PROTEIN; CHAIN: A;				TOLB PROTEIN; CHAIN: A;			TOI B PROTEIN: CHAIN: 4:	יה יווחויי, טובווטוי ה'
Table 5	SEQ FOLD											*******										
Ta	PMF			0.40			86:0				06.0			99.0				0.15			0.04	10.01
	Verify score			0.12			0.45				80.0			0.13				0.49			80 O-	2
	Psi Blast			0.0012			1.2e-33				0.00051			6e-07				5.1e-05			6.80-05	20.00
	END AA			113			339				218			243				764			876	
	START AA			23			99				107			111		•		564		_	674	
	CHAIN										A			A				¥			A	
	PDB ID			2bnh			2bnh			74	1crz		•	1crz				1crz	•		1crz.	7
	S			1621			1621	*****			1623			1623				1623			1623	1

					* *		저 —-	I _K		*		×		Ä		K K		K.) <u>R</u>)R)R				A			
	PDB annotation		TWO DOMAINS: BETA PROPELLER AND	ALPHA/BETA FOLD	TRANSCRIPTION INHIBITOR	BETA-PROPELLER	TRANSCRIPTION INHIBITOR BETA-PROPELLER	TRANSCRIPTION INHIBITOR	BETA-PROPELLER	COMPLEX (GTP-	BINDING/TRANSDUCER)	BETA1, TRANSDUCIN BETA	SUBUNIT; GAMMA1,	TRANSDUCIN GAMMA	SUBUNIT; COMPLEX (GTP-																
			TWO DC	ALPHA	TRANSC	BEIA-PI	TRANSC BETA-PI	TRANSC	BETA-PI	COMPLI	BINDIN	BETA1,	SUBUNI	TRANSI	SUBUNI																
	Compound				TRANSCRIPTIONAL REPRESSOR	IUPI; CHAIN: A, B, C;	TRANSCRIPTIONAL REPRESSOR	TRANSCRIPTIONAL REPRESSOR	TUP1; CHAIN: A, B, C;	TRANSCRIPTIONAL REPRESSOR	TUP1; CHAIN: A, B, C;	TRANSCRIPTIONAL REPRESSOR	TUP1; CHAIN: A, B, C;	TRANSCRIPTIONAL REPRESSOR	TUP1; CHAIN: A, B, C;	TRANSCRIPTIONAL REPRESSOR	TUP1; CHAIN: A, B, C;	TRANSCRIPTIONAL REPRESSOR	TUP1; CHAIN: A, B, C;	TRANSCRIPTIONAL REPRESSOR	TUP1; CHAIN: A, B, C;	TRANSCRIPTIONAL REPRESSOR	TUP1; CHAIN: A, B, C;	TRANSCRIPTIONAL REPRESSOR	TUP1; CHAIN: A, B, C;	GT-ALPHA/GI-ALPHA CHIMERA;	CHAIN: A; GT-BETA; CHAIN: B;	GT-GAMMA; CHAIN: G;			
Table 5	SEQ	FOLD																													
Ta	PMF	score			-0.20		0.24	0.24		0.84		-0.09		1.00		-0.06		0.31		0.59		-0.11		-0.15		0.83					
	Verify	score			60.0		0.11	0.31		0.42		0.43		0.41		0.23		0.33		0.28		0.20		0.04		0.52					
	Psi	Blast			1.5e-60		2e-17	3.4e-60		1.2e-47		3.4e-57		3.4e-58		3.4e-58		(e-31		1e-61		1e-61		5.1e-58		3.4e-54					
	END:	AA			1291	,	646	523		224		562		344		059		813		856		949		994		441					
	START	AA			1012		153	190		2		251		31		339		364		572		999		700		105					
	CHAIN				А		⋖	A		A		A		A		Ą		Ą		Ą		А	ĺ	А		В					
	PDB	a			1erj		lerj	1erj		lerj		1erj		lerj		1got															
	SEQ	NO.			1623		1623	1623		1623		1623		1623		1623		1623		1623	ļ	1623		1623		1623					

	PDB annotation	BINDING/TRANSDUCER), G PROTEIN, HETEROTRIMER 2 SIGNAL TRANSDUCTION	COMPLEX (GTP- BINDING/TRANSDUCER) BETA1, TRANSDUCIN BETA	SUBUNIT; GAMMA1, TRANSDUCIN GAMMA	BINDING/TRANSDUCER), G PROTEIN, HETEROTRIMER 2 SIGNAL TRANSDUCTION	COMPLEX (GTP- BINDING/TRANSDUCER) BETAL TRANSDUCIN BETA	SUBUNIT; GAMMA1,	SUBUNIT; COMPLEX (GTP-	BINDING/TRANSDUCER), G PROTEIN, HETEROTRIMER 2	SIGNAL TRANSDUCTION	COMPLEX (GTP-BINDING/TRANSDUCER)	BETA1, TRANSDUCIN BETA	SUBUNIT; GAMMAI,	TRANSDUCIN GAMMA SUBINITY COMPLEX (GTP-	BINDING/TRANSDUCER), G	PROTEIN, HETEROTRIMER 2 SIGNAL TRANSDUCTION	1	
	Compound		GT-ALPHA/GI-ALPHA CHIMERA; CHAIN: A; GT-BETA; CHAIN: B; GT-GAMMA: CHAIN: G:	O'-Charles, Circuit, C.		GT-ALPHA/GI-ALPHA CHIMERA; CHAIN: A; GT-BETA; CHAIN: B; GT GAMMA: CHAIN: G:	OI-OMMIN, CLIMAN C,	·			GT-ALPHA/GI-ALPHA CHIMERA;	GT-GAMMA; CHAIN: G;					GT-ALPHA/GI-ALPHA CHIMERA;	
Table 5	SEQ FOLD score																	
Tak	PMF score		0.10			0.75					0.74						0.40	;
	Verify score		0.30			0.10					0.36						0.24	- 1
	Psi Blast		6.8e-56			1.4e-19					5.1e-69						1 4e-49	11.71.1
	END		559			695					282						648	010
	START		239			299		·			3						345	040
	CHAIN		В			В					B						P	α
	PDB ID		1got			1got					1got			×			1	lgot
	SEQ ID	Ö	1623			1623					1623						57,	1623

																			1
	PDB annotation	BINDING/TRANSDUCER) BETA1, TRANSDUCIN BETA SUBUNIT; GAMMA1, TRANSDUCIN GAMMA	SUBUNIT; COMPLEX (GTP-BINDING/TRANSDUCER), GPROTEIN, HETEROTRIMER 2 SIGNAL TRANSDUCTION	COMPLEX (GTP-BINDING/TRANSDUCER)	SUBUNIT; GAMMAI,	TRANSDUCIN GAMMA SUBUNIT: COMPLEX (GTP-	BINDING/TRANSDUCÈR), G	PROTEIN, HETEROTRIMER 2	COMPLEX (GTP-	BINDING/TRANSDUCER)	BETAL, TRANSDUCIN BETA SUBUNIT; GAMMAI,	TRANSDÚCIN GAMMA	SUBUNIT; COMPLEX (GTP-	BINDING/TRANSDUCER), G	SIGNAL TRANSDUCTION	COMPLEX (GTP-BINDING/TRANSDUCER)	BETA1, TRANSDUCIN BETA	SUBUNTI; GAMMAI, TRANSDUCIN GAMMA	
	Compound	CHAIN: A; GT-BETA; CHAIN: B; GT-GAMMA; CHAIN: G;		GT-ALPHA/GI-ALPHA CHIMERA; CHAIN: A; GT-BETA; CHAIN: B;	GT-GAMMA; CHAIN: G;				GT-ALPHA/GI-ALPHA CHIMERA;	CHAIN: A; GT-BETA; CHAIN: B;	GT-GAMMA; CHAIN: G;					GT-ALPHA/GI-ALPHA CHIMERA; CHAIN: A: GT-BETA: CHAIN: B:	GT-GAMMA; CHAIN: G;		
Table 5	SEQ FOLD score																		
Tal	PMF score			0.34	·····				0.05							0.49			
	Verify score	-		0.12					0.38		411.0					0.41			
	Psi Blast			6.8e-51					8e-23							8.5e-70			
	END AA			695					813							853			
	START			398					494						•	563			
	CHAIN			В					В							В			
	PDB ID			lgot					1got)		-				1got			
	SEQ ID			1623		-			1623							1623	_		

	PDB annotation	SUBUNIT; COMPLEX (GTP-BINDING/TRANSDUCER), GPROTEIN, HETEROTRIMER 2 SIGNAL TRANSDUCTION	COMPLEX (GTP-BINDING/TRANSDUCER) BETA1, TRANSDUCIN BETA SUBUNIT; GAMMA1, TRANSDUCIN GAMMA SUBUNIT; COMPLEX (GTP-BINDING/TPANSDUCIN) G	PROTEIN, HETEROTRIMER 2 SIGNAL TRANSDUCTION	COMPLEX (GTP- BINDING/TRANSDUCER) BETA1, TRANSDUCIN BETA	SUBUNIT; GAMMA1, TRANSDUCIN GAMMA STIBINIT: COMPIEX (GTP.	BINDING/TRANSDUCER), G	FRUIEIN, HEIERUIRIMER 2 SIGNAL TRANSDUCTION	COMPLEX (GTP- BINDING/TRANSDUCER) BETA1, TRANSDUCIN BETA	SUBUNIT; GAMMAI,	SUBUNIT; COMPLEX (GTP-	BINDING/TRANSDUCER), G	PROTEIN, HETEROTRIMER 2 SIGNAL TRANSDUCTION
	Compound		GT-ALPHA/GI-ALPHA CHIMERA; CHAIN: A; GT-BETA; CHAIN: B; GT-GAMMA; CHAIN: G;		GT-ALPHA/GI-ALPHA CHIMERA; CHAIN: A; GT-BETA; CHAIN: B; GT-GAMMA; CHAIN: G;				GT-ALPHA/GI-ALPHA CHIMERA; CHAIN: A; GT-BETA; CHAIN: B; GT-GAMMA: CHAIN: G:				
Table 5	SEQ FOLD score												
Tac	PMF		0.71		-0.15				-0.18				
	Verify score		0.50		0.15				0.06				
	Psi Blast		1.7e-61		3.4e-60				1.7e-65				
	END		387		950	_			1041				
	START		09		655				745				
	CHAIN ID		æ		В				В				
	PDB ID		1got		lgot				Igot				
	SEQ DO		1623		1623				1623				

	PDB annotation		TRANSFERASE BROMODOMAIN, HISTONE-ACETYLTRANSFERASE, NMR-STRUCTURE	GENE REGULATION BROMODOMAIN, HISTONE BINDING, N-ACETYL LYSINE	TRANSCRIPTION TAFII250; FOUR-HELIX BUNDLE, ACETYLATED HISTONE- TAIL BINDING PROTEIN	TRANSCRIPTION TAFII250; FOUR-HELIX BUNDLE, ACETYLATED HISTONE- TAIL BINDING PROTEIN	COMPLEX (ZINC FINGER/DNA) COMPLEX (ZINC FINGER/DNA), ZINC FINGER, DNA-BINDING PROTEIN	COMPLEX (ZINC FINGER/DNA) COMPLEX (ZINC FINGER/DNA), ZINC FINGER, DNA-BINDING PROTEIN	COMPLEX (ZINC FINGER/DNA) COMPLEX (ZINC FINGER/DNA), ZINC
	Compound		HISTONE ACETYLTRANSFERASE; CHAIN: A;	TRANSCRIPTIONAL ACTIVATOR GCN5; CHAIN: A; H4 PEPTIDE; CHAIN: P;	RNA POLYMERASE II TRANSCRIPTION INITIATION CHAIN: A;	RNA POLYMERASE II TRANSCRIPTION INITIATION CHAIN: A;	QGSR ZINC FINGER PEPTIDE; CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE; CHAIN: B, C;	QGSR ZINC FINGER PEPTIDE; CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE; CHAIN: B, C;	QGSR ZINC FINGER PEPTIDE; CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING
Table 5	SEQ FOLD score								
Tal	PMF	,	1.00	96.0	0.51	0.90	0.49	1.00	1.00
	Verify score		0.40	0.03	0.01	-0.26	0.20	0.29	0.29
	Psi Blast		1.7e-27	3.4e-29	1e-22	2e-20	5.1e-17	1.2e-26	8e-36
	END		153	154	151	239	199	227	256
	START AA		42	54	24	58	140	148	175
	CHAIN		A	A	A	A	A	А	Ą
	PDB ID		1691	1e6i	leqf	1eqf	lalh	lalh	lalh
	SEQ Signal		1624	1624	1624	1624	1631	1631	1631

	PDB annotation	FINGER, DNA-BINDING PROTEIN	COMPLEX (ZINC	FINGER/DNA) COMPLEX	(ZINC FINGER/DNA), ZINC	FINGER, DNA-BINDING	PROTEIN	COMPLEX (ZINC	FINGER/DNA) COMPLEX	(ZINC FINGER/DNA), ZINC	FINGER, DNA-BINDING	PROTEIN	COMPLEX (ZINC	FINGER/DNA) COMPLEX	(ZINC FINGER/DNA), ZINC	FINGER, DNA-BINDING	PROTEIN	CONTRACTILE LIM	DOMAIN, CRP, NMR,	MUSCLE DIFFERENTIATION,	CONTRACTILE	COMPLEX (ZINC	FINGER/DNA) ZINC FINGER,	PROTEIN-DNA	INTERACTION, PROTEIN	DESIGN, 2 CRYSTAL	STRUCTURE, COMPLEX	(ZINC FINGER/DNA)	COMPLEX (ZINC	FINGER/DNA) ZINC FINGER,	PROTEIN-DNA
	Compound	SITE; CHAIN: B, C;	QGSR ZINC FINGER PEPTIDE;	CHAIN: A; DUPLEX	OLIGONUCLEOTIDE BINDING	SITE; CHAIN: B, C;		QGSR ZINC FINGER PEPTIDE;	CHAIN: A; DUPLEX	OLIGONUCLEOTIDE BINDING	SITE; CHAIN: B, C;		QGSR ZINC FINGER PEPTIDE;	CHAIN: A; DUPLEX	OLIGONUCLEOTIDE BINDING	SITE; CHAIN: B, C;		CRP1; CHAIN: A;				DNA; CHAIN: A, B, D, E;	CONSENSUS ZINC FINGER	PROTEIN; CHAIN: C, F, G;					DNA; CHAIN: A, B, D, E;	CONSENSUS ZINC FINGER	PROTEIN; CHAIN: C, F, G;
lable 5	SEQ FOLD score												77.27					59.99													
La	PMF score		1.00					1.00														1.00			**				1.00		
	Verify score		0.27					0.17														60.0							0.40		
	Psi Blast	•	2e-36					1.4e-35					1.4e-35					8e-14				8.5e-29							1.4e-46		
	END		284					396					397					337				199							227		
	START		204					315					315					141				142	٠						146		
	CHAIN ID		A					A					A					A				ပ							2		
	PDB ID		lalh					lalh					1a1h					1b8t				1mey				-			1mey		
	SEQ NO:		1631					1631					1631					1631				1631			-				1631		

					,	
	PDB annotation	INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA)	COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA)	COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA)	COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA)	COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX
	Compound		DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G;	DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G;	DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G;	DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER PROTEIN; CHAIN: C, F, G;
Table 5	SEQ FOLD score			89.86		
Tal	PMF score		1.00		1.00	1.00
	Verify score		0.16		0.31	0.10
	Psi Blast		6.8e-50	1.7e-51	1.7e-51	5.1e-51
	END		255	256	283	311
	START		174	174	202	230
	CHAIN		U	O	O	O
	PDB ID		Imey	1теу	1mey	1mey
	SEQ No.		1631	1631	1631	1631

4	PDB annotation		(ZINC FINGER/DNA)	COMPLEX (ZINC FINGER, FINGER, ZINC FINGER,	PROTEIN-DNA	INTERACTION, PROTEIN	DESIGN, 2 CRYSTAL	STRUCTURE, COMPLEX (ZINC FINGER/DNA)	COMPLEX (ZINC FINGER.	PROTEIN-DNA	INTERACTION, PROTEIN	DESIGN, 2 CRYSTAL	STRUCTURE, COMPLEX	(ZINC FINGER/DNA)	COMPLEX (ZINC	FINGER/DNA) ZINC FINGER,	PROTEIN-DNA	INTERACTION, PROTEIN	DESIGN, 2 CRYSTAL	STRUCTURE, COMPLEX	(ZINC FINGER/DNA)	COMPLEX (ZINC	FINGER/DNA) ZINC FINGER,	PROTEIN-DNA	INTERACTION, PROTEIN	DESIGN, 2 CRYSTAL	STRUCTURE, COMPLEX	(ZINC FINGER/DNA)	COMPLEX (TRANSCRIPTION REGULATION/DNA) TFIIIA;	
	Compound			DNA; CHAIN: A, B, D, E; CONSENSUS ZINC FINGER	PROTEIN; CHAIN: C, F, G;				DNA; CHAIN: A, B, D, E;	PROTEIN; CHAIN: C, F, G;					DNA; CHAIN: A, B, D, E;	CONSENSUS ZINC FINGER	PROTEIN; CHAIN: C, F, G;					DNA; CHAIN: A, B, D, E;	CONSENSUS ZINC FINGER	PROTEIN; CHAIN: C, F, G;	-				TRANSCRIPTION FACTOR IIIA; CHAIN: A; 5S RNA GENE;	, , , , , , , , , , , , , , , , , , , ,
Table 5	SEQ	I OLD score																					-							
Ta	PMF	score		66.0					1.00						0.74							0.43							0.07	
	Verify	score		-0.26					90.0						90.0							0.70							0.34	
	Psi	Blast		1.4e-46					1.7e-38						8.5e-49							5.1e-09							5.1e-11	
	END	ΑA		367					395						426							171							195	
•	START	AA		258				-	314						342	!						144							143	
	CHAIN	<u>a</u>		C					O O						S)						٣)						A	
	PDB	А		1mey					1mey						1mev							1mev							1463	
	SEQ	요 S	į.	1631					1631						1631							1631							1631	

	PDB annotation		5S GENE; NMR, TFIIIA, PROTEIN, DNA,	TRANSCRIPTION FACTOR,	5S RNA 2 GENE, DNA	BINDING PROTEIN, ZINC	FINGER, COMPLEX 3	(TRANSCRIPTION REGIT ATTON/DNA)	COMPLEX (TRANSCRIPTION	REGULATION/DNA) TFIIIA;	5S GENE; NMR, TFIIIA,	PROTEIN, DNA,	TRANSCRIPTION FACTOR,	5S RNA 2 GENE, DNA	BINDING PROTEIN, ZINC	FINGER, COMPLEX 3	(TRANSCRIPTION	REGULATION/DNA)	COMPLEX (TRANSCRIPTION	REGULATION/DNA)	COMPLEX (TRANSCRIPTION	REGULATION/DNA), RNA	POLYMERASE III, 2	TRANSCRIPTION	INITIATION, ZINC FINGER	PROTEIN	COMPLEX (TRANSCRIPTION PEGIT ATTON/DNA)	COMPLEX (TRANSCRIPTION	REGULATION/DNA), RNA	POLYMERASE III, 2
	Compound		CHAIN: E, F;						TRANSCRIPTION FACTOR IIIA:	CHAIN: A; 5S RNA GENE;	CHAIN: E, F;								TFIIIA; CHAIN: A, D; 5S	RIBOSOMAL RNA GENE; CHAIN:	B, C, E, F;						TFIIIA; CHAIN: A, D; 5S	NECOCIATE MAN CENE, CLERK.	D, C, L, I,	
Table 5	SEQ	FOLD																	108.16											
Tat	PMF	score							06.0)																	1.00	•		
	Verify	score							0.47	: ;																	80.0			
	Psi	Blast							6.88-20										4e-59								1.5e-37			
	END	AA —						,	777	1									314								292			
	START	AA							147	\ 									146								147			
	CHAIN	<u> </u>								¢									A	:							A			
	PDB	<u> </u>			•				1+5	3									1tf6								1tf6			
	SEQ	A È							1631	1001			-						1631	())							1631			

																т		7
	PDB annotation	TRANSCRIPTION INITIATION, ZINC FINGER PROTEIN	COMPLEX (TRANSCRIPTION REGULATION/DNA) COMPLEX (TRANSCRIPTION BRIGHT ATTOMINAL BRIGHT)	KEGULA HON/DNA), KNA POLYMERASE III, 2 TRANSCRIPTION INITIATION, ZINC FINGER PROTEIN	COMPLEX (TRANSCRIPTION	KEGULATION/DNA) COMPLEX (TRANSCRIPTION	REGULATION/DNA), RNA POLYMERASE III. 2	TRANSCRIPTION	INITIATION, ZINC FINGER	PROTEIN	COMPLEX (TRANSCRIPTION REGULATION DNA)	COMPLEX (TRANSCRIPTION	KEGULA HOM/DINA), KINA POLYMERASE III, 2	TRANSCRIPTION	INITIATION, ZINC FINGER PROTEIN	COMPLEX (TRANSCRIPTION	REGULATION/DNA) COMPLEX (TRANSCRIPTION	KEGULAHON/DINA), KANA
	Compound		TFIIIA; CHAIN: A, D; 5S RIBOSOMAL RNA GENE; CHAIN: B, C, E, F;		TFIIIA; CHAIN: A, D; 5S	KIBOSOMAL KNA GENE; CHAIN: B, C, E, F;					TFIIIA; CHAIN: A, D; 5S RIBOSOMAL RNA GENE; CHAIN:	B, C, E, F;				TFIIIA; CHAIN: A, D; 5S	RIBOSOMAL RNA GENE; CHAIN: B, C, E, F;	
Table 5	SEQ FOLD score																	
Tat	PMF		96.0		1.00						1.00					1.00		
	Verify score		-0.10		-0.11						-0.21					-0.14		
	Psi Blast		4e-42		4e-58						4e-59					8e-59		
	END		283		339						367					395		
	START		153		175						204					231		
	CHAIN ID		А		A						Y					A		
	PDB ID		1tf6		1tf6						1tf6					146		
	SEQ F)	2	1631		1631						1631					1631		

	PDB annotation		POLYMERASE III, 2 TRANSCRIPTION INITIATION, ZINC FINGER	PROTEIN	COMPLEX (TRANSCRIPTION REGULATION/DNA)	COMPLEX (TRANSCRIPTION	REGULATION/DNA), RNA	FOLTMERASE III, Z TRANSCRIPTION	INITIATION, ZINC FINGER	PROTEIN	COMPLEX (TRANSCRIPTION	REGULATION/DNA)	COMPLEX (TRANSCRIPTION	REGULATION/DNA), RNA	POLYMERASE III, 2	TRANSCRIPTION	INITIATION, ZINC FINGER	PROTEIN	COMPLEX (TRANSCRIPTION	REGULATION/DNA) YING-	YANG 1; TRANSCRIPTION	INITIATION, INITIATOR	ELEMENT, YY1, ZINC 2	FINGER PROTEIN, DNA-	PROTEIN RECOGNITION, 3	COMPLEX (TRANSCRIPTION	REGULATION/DNA)	COMPLEX (TRANSCRIPTION	KEGULATION/DINA) TING-
	Compound				TFIIIA; CHAIN: A, D; 5S RIBOSOMAI, RNA GENE: CHAIN:	B, C, E, F;					TFIIIA; CHAIN: A, D; 5S	RIBOSOMAL RNA GENE; CHAIN:	B, C, E, F;						YY1; CHAIN: C; ADENO-	ASSOCIATED VIRUS P5	INITIATOR ELEMENT DNA;	CHAIN: A. B.						YY1; CHAIN: C; ADENO-	ASSOCIATED VIRUS PS
Table 5	SEQ FOLD	score				_																						85.96	
Tak	PMF score				1.00						0.35								1.00										
	Verify score				-0.28						-0.28								0.24										
	Psi Blast				8.5e-34						1.4e-31								1.2e-28									1.8e-43	
	END				409						453	!							227									256	
	START				259			•			287								141									149	
	CHAIN				A						4	4							C	,								O	
	PDB ID				1tf6						1+66	211							liihd									1ubd	
	SEQ	ĊN			1631		1				1631								1631									1631	

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Table 5	
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	PDB annotation	YANG 1; TRANSCRIPTION INITIATION, INITIATOR ELEMENT, YY1, ZINC 2 FINGER PROTEIN, DNA- PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULATION/DNA)	COMPLEX (TRANSCRIPTION REGULATION/DNA) YING-YANG 1; TRANSCRIPTION INITIATOR INITIATION, INITIATOR ELEMENT, YY1, ZINC 2 FINGER PROTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULATION/DNA)	COMPLEX (TRANSCRIPTION REGULATION/DNA) YING-YANG 1; TRANSCRIPTION INTIATION INTIATION ELEMENT, YY1, ZINC 2 FINGER PROTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULATION/DNA)	COMPLEX (TRANSCRIPTION REGULATIONDNA) YING- YANG 1; TRANSCRIPTION INITIATION, INITIATOR ELEMENT, YY1, ZINC 2 FINGER PROTEIN, DNA-
	Compound	INITIATOR ELEMENT DNA; CHAIN: A, B;	YY1; CHAIN: C; ADENO- ASSOCIATED VIRUS P5 INITIATOR ELEMENT DNA; CHAIN: A, B;	YY1; CHAIN: C; ADENO- ASSOCIATED VIRUS P5 INITIATOR ELEMENT DNA; CHAIN: A, B;	YY1; CHAIN: C; ADENO- ASSOCIATED VIRUS P5 INITIATOR ELEMENT DNA; CHAIN: A, B;
Table 5	SEQ FOLD score				
Tat	PMF		1.00	1.00	1.00
	Verify score		0.11	0.10	0.36
	Psi Blast		8e-36	1e-33	1.8e-43
	END		255	255	283
	START		151	154	178
	CHAIN ID		O	O	S
	PDB ID		lubd	1ubd	1ubd
	SEQ EQ		1631	1631	1631

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	PDB annotation		PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULATION/DNA)	COMPLEX (TRANSCRIPTION	KEGULA HON/DINA) TING- YANG 1; TRANSCRIPTION	INITIATION, INITIATOR	ELEMENT, YY1, ZINC 2 FINGER PROTEIN DNA-	PROTEIN RECOGNITION, 3	COMPLEX (TRANSCRIPTION	KEGULATION/DINA)	COMPLEX (IRANSCRIPTION	REGULATION/DNA) YING-	YANG I; TRANSCRIPTION	INITIATION, INITIATOR	ELEMENT, YY1, ZINC 2	FINGER PROTEIN, DNA-	PROTEIN RECOGNITION, 3	COMPLEX (TRANSCRIPTION	REGULATION/DNA)	COMPLEX (TRANSCRIPTION	REGULATION/DNA) YING-	YANG 1; TRANSCRIPTION	INITIATION, INITIATOR	ELEMENT, YY1, ZINC 2	FINGER PROTEIN, DNA-	PROTEIN RECOGNITION, 3	COMPLEX (TRANSCRIPTION	REGULATION/DNA)	COMPLEX (TRANSCRIPTION	
	Compound			YY1; CHAIN: C; ADENO-	ASSOCIATED VIRUS PS INITIATOR ELEMENT DNA:	CHAIN: A. B.					YY1; CHAIN: C; ADENO-	ASSOCIATED VIRUS P5	INITIATOR ELEMENT DNA;	CHAIN: A, B;						YY1; CHAIN: C; ADENO-	ASSOCIATED VIRUS P5	INITIATOR ELEMENT DNA;	CHAIN: A. B:						YY1; CHAIN: C; ADENO-	1
Table 5	SEQ	FULD	-																							****				
Tat	PMF	score		1.00							1.00									0.71									1.00	
	Verify	score		0.14							0.09									-0.24									-0.06	
	Psi	Blast		1.5e-35							8e-46									1.2e-30	2								8e-45	
	END	AA		311							340									305)								395	
	START	AA		210							228								•	996	202								284	
	CHAIN	А		O							C	1								ر	د								O	
	PDB	<u> </u>		1ubd							lubd				-				-	1.150	noni								1ubd	2022
	SEQ	 ⊖ Ş	5	1631							1631	1								1631	1001								1631	1 2 1

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|         | PDB annotation       | REGULATION/DNA) YING-<br>YANG 1; TRANSCRIPTION<br>INITIATION, INITIATOR | ELEMENT, YY1, ZINC 2 | PROTEIN RECOGNITION, 3 | COMPLEX (TRANSCRIPTION REGULATION/DNA) | COMPLEX (DNA-BINDING         | PROTEIN/DNA) FIVE-          | FINGER GLI; GLI, ZINC<br>ENGEP COMPI EX (DNA. | BINDING PROTEIN/DNA)                      | COMPLEX (DNA-BINDING | PROTEIN/DNA) FIVE-               | FINGER GLI; GLI, ZINC | FINGER, COMPLEX (DNA- | BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING        | PROTEIN/DNA) FIVE-          | FINGER GLI; GLI, ZINC | INGER, COMPLEX (DNA- | BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING | PROTEIN/DNA) FIVE-          | FINGER GLI; GLI, ZINC | FINGER, COMPLEX (DNA- | BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING      | PROTEIN/DNA) FIVE- | FINGER GLI; GLI, ZINC |
|---------|----------------------|-------------------------------------------------------------------------|----------------------|------------------------|----------------------------------------|------------------------------|-----------------------------|-----------------------------------------------|-------------------------------------------|----------------------|----------------------------------|-----------------------|-----------------------|----------------------|-----------------------------|-----------------------------|-----------------------|----------------------|----------------------|----------------------|-----------------------------|-----------------------|-----------------------|----------------------|---------------------------|--------------------|-----------------------|
|         | Compound             | ASSOCIATED VIRUS P5 INITIATOR ELEMENT DNA; CHAIN: A. B;                 |                      | FL PF                  | CC                                     | ZINC FINGER PROTEIN GLII; CO | CHAIN: A; DNA; CHAIN: C, D; | FI                                            | H. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. |                      | CHAIN: A; DNA; CHAIN: C, D;   PI |                       | 田<br>                 | B                    | ZINC FINGER PROTEIN GLII; C | CHAIN: A; DNA; CHAIN: C, D; |                       | <u> </u>             |                      |                      | CHAIN: A; DNA; CHAIN: C, D; |                       | <u> </u>              | <u>8</u>             | ZINC FINGER PROTEIN GLII; |                    |                       |
| Table 5 | SEQ<br>FOLD<br>score |                                                                         |                      |                        |                                        |                              |                             |                                               |                                           |                      |                                  | -                     |                       |                      |                             |                             |                       |                      |                      | 92.55                |                             |                       |                       |                      |                           |                    |                       |
| Tab     | PMF<br>score         |                                                                         |                      |                        |                                        | 0.99                         |                             |                                               |                                           | 86.0                 |                                  |                       |                       |                      | 1.00                        |                             |                       |                      |                      |                      |                             |                       |                       |                      | 1.00                      |                    |                       |
|         | Verify               |                                                                         |                      |                        |                                        | 0.07                         |                             |                                               |                                           | -0.02                |                                  |                       |                       |                      | 0.31                        |                             |                       |                      |                      |                      |                             |                       |                       |                      | 0.13                      |                    |                       |
|         | Psi<br>Blast         |                                                                         |                      |                        |                                        | 4e-38                        |                             |                                               |                                           | 1e-34                |                                  |                       |                       |                      | 8e-57                       |                             |                       |                      |                      | 4e-59                |                             |                       |                       |                      | 4P-50                     | 2                  |                       |
|         | END                  |                                                                         |                      |                        |                                        | 285                          |                             |                                               |                                           | 282                  |                                  |                       |                       |                      | 313                         | 1                           |                       |                      |                      | 341                  | !<br>!                      |                       |                       |                      | 360                       | )<br>              |                       |
|         | START                |                                                                         |                      |                        |                                        | 151                          |                             |                                               |                                           | 154                  |                                  |                       |                       |                      | 175                         | )<br>-                      |                       |                      |                      | 200                  | 9                           |                       |                       |                      | 200                       | 707                |                       |
|         | CHAIN                |                                                                         |                      |                        | · · · ·                                | <b>V</b>                     | 17                          |                                               |                                           | A                    |                                  |                       |                       |                      | A                           | 4                           |                       |                      |                      | A                    | 7.7                         | _                     |                       |                      |                           | <u>د</u>           |                       |
|         | PDB<br>ID            |                                                                         |                      |                        |                                        | 2ali                         | 72911                       |                                               |                                           | 20li                 | i<br>a                           |                       |                       |                      | 2oli                        | 78m                         |                       |                      |                      | Joli                 | 72m                         |                       |                       |                      | 221:                      | 1187               |                       |
|         | SEQ<br>U             |                                                                         |                      |                        |                                        | 1631                         | 1001                        |                                               |                                           | 1631                 |                                  |                       |                       |                      | 1631                        | 1001                        |                       |                      |                      | 1631                 | 1001                        |                       |                       |                      | 1631                      | 1001               |                       |

| e 5           |  |
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| $\frac{a}{b}$ |  |
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|         | Compound PDB annotation |         | FINGER, COMPLEX (DNA-BINDING PROTEIN/DNA) | ZINC FINGER PROTEIN GLII; COMPLEX (DNA-BINDING | CHAIN: A; DNA; CHAIN: C, D; PROTEIN/DNA) FIVE- | FINGER GLI; GLI, ZINC | FINGER, COMPLEX (DNA- | BINDING PROTEINDNA) | ZINC FINGER PROTEIN GLII; COMPLEX (DNA-BINDING |              | FINGER, COMPLEX (DNA- | BINDING PROTEIN/DNA) | OMPK36; CHAIN: A, B, C; OUTER MEMBRANE PROTEIN OSMOPORIN: | OITTER MEMBRANE | PROTEIN NON-SPECIFIC | PORIN, OSMOPORIN, 2 | BETA-BARREL. | TRANSMEMBRANE | METHYLMALONYL-COA ISOMERASE ISOMERASE, | MUTASE; CHAIN: A, B, C, D; MUTASE, | INTRAMOLECULAR | TRANSFERASE | DNA-BINDING PROTEIN | ANTENNAFEDIA FROTEIN<br>(HOMFODOMAIN) MITTANT | WITH CYS 39 1AHD 3 REPLACED | BY SER (C39S) COMPLEX WITH |               |
|---------|-------------------------|---------|-------------------------------------------|------------------------------------------------|------------------------------------------------|-----------------------|-----------------------|---------------------|------------------------------------------------|--------------|-----------------------|----------------------|-----------------------------------------------------------|-----------------|----------------------|---------------------|--------------|---------------|----------------------------------------|------------------------------------|----------------|-------------|---------------------|-----------------------------------------------|-----------------------------|----------------------------|---------------|
|         | O                       |         |                                           | ZINC FINGER                                    | CHAIN: A; DI                                   |                       |                       |                     | ZINC FINGEL                                    | CILMIN: A, D |                       |                      | OMPK36; CH                                                |                 |                      |                     |              |               | METHYLMA                               | MUTASE; CI                         |                |             | DNA-BINDIN          | (HOMEODO                                      | WITH CYS 3                  | BY SER (C39S) COMPL        | לידיייין טיוט |
| Table 5 | SEQ                     | FOLD    |                                           |                                                |                                                |                       |                       |                     |                                                |              |                       |                      |                                                           |                 |                      |                     |              |               |                                        |                                    |                |             |                     |                                               |                             |                            |               |
| Tal     | PMF                     | score   |                                           | 1.00                                           |                                                |                       |                       |                     | 0.19                                           |              |                       |                      | -0.20                                                     |                 |                      |                     |              |               | -0.18                                  | )<br>;                             |                |             | 0.13                |                                               |                             |                            |               |
|         | Verify                  | score   |                                           | 0.14                                           |                                                |                       |                       |                     | -0.15                                          |              |                       |                      | 0.84                                                      |                 |                      |                     |              |               | 0.22                                   | 1                                  |                |             | 0.38                |                                               |                             |                            |               |
|         | Psi                     | Blast   |                                           | 1e-57                                          |                                                |                       |                       |                     | 3.4e-32                                        |              |                       |                      | 2.2e-08                                                   |                 |                      |                     |              |               | 2 26-10                                |                                    |                |             | 1.7e-27             |                                               |                             |                            |               |
|         | END                     | ΑA      |                                           | 396                                            | )<br>)                                         |                       |                       |                     | 455                                            |              |                       |                      | 212                                                       |                 |                      |                     |              |               | 581                                    | 5                                  |                |             | 166                 |                                               |                             |                            |               |
|         | START                   | AA      |                                           | 258                                            | 2                                              |                       |                       |                     | 294                                            |              |                       |                      | 18                                                        |                 |                      |                     |              |               | 787                                    | È                                  |                |             | 100                 |                                               |                             |                            |               |
|         | CHAIN                   | <u></u> |                                           | A                                              | <b>4</b>                                       |                       |                       |                     | A                                              |              |                       |                      | A                                                         |                 |                      |                     |              |               | <                                      | τ                                  |                |             | Ь                   |                                               |                             |                            |               |
|         | PDB                     |         |                                           | 20%                                            | 7 P                                            |                       |                       |                     | 2gli                                           |              |                       |                      | losm                                                      |                 |                      |                     |              |               | 1                                      | 1311<br>                           |                |             | 1ahd                |                                               |                             |                            |               |
|         | SEQ                     | ВŞ      |                                           | 1631                                           | 1001                                           |                       |                       |                     | 1631                                           |              |                       |                      | 1644                                                      |                 |                      |                     |              |               | 1644                                   | †<br>101<br>101                    |                |             | 1645                |                                               |                             |                            |               |

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|---------|----------------|-------|--------------------|---------------------------------------------|----------------------|--------------------------------------------------------|------------------------------------------|--------------------------|-------------------------------|----------------------------------------------|--------------------------|-------------------------------|-------------------------|----------------------|------------------------|-----------------------|------------------------|--------------------------|-----------------------------|--------------------------------|--------------------------|-----------------------|-----------------------|--------------------------|-----------------------------|----------------|-------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
|         | PDB annotation |       |                    |                                             |                      |                                                        |                                          | PROTEIN/DNA              | HOMEODOMAIN, DNA,             | COMPLEX, DNA-BINDING<br>PROTEIN, PROTEIN/DNA | PROTEIN/DNA              | HOMEODOMAIN, DNA,             | COMPLEX, DNA-BINDING    | PROTEIN, PROTEIN/DNA | TRANSCRIPTION/DNA      | DEPOTED DIN BINDING   | FROIEIN, DINA BINDING, | HOMEODOMAIN,             | HOMEOTIC FROIEINS,          | DEVELOTIVE 1, 2<br>SPECIFICITY | TRANSCRIPTION/DNA        | ULTRABITHORAX; PBX    | PROTEIN; DNA BINDING, | HOMEODOMAIN,             | HOMEOTIC PROTEINS,          | DEVELOPMENT, 2 | TRANSCRIPTION/DNA       |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |
|         | Compound       |       | STRUCTURES) 1AHD 5 | DNA-BINDING PROTEIN<br>ANTENNAPEDIA PROTEIN | (HOMEODOMAIN) MUTANT | WITH CYS 39 1AHD 3 KEPLACED RY SER (C39S) COMPLEX WITH | DIA (NMR, 1AHD 4 16<br>STRICTHES) 1AHD 5 | HOMEOBOX PROTEIN HOX-B1; | CHAIN: A; PBX1; CHAIN: B; DNA | CHAIN: D; DNA CHAIN: E;                      | HOMEOBOX PROTEIN HOX-B1; | CHAIN: A; PBX1; CHAIN: B; DNA | CHAIN: D; DNA CHAIN: E; |                      | ULTRABITHORAX HOMEOTIC | FROIEIN IV; CHAIN: A; | HOMEOBOX PROTEIN       | EXTRADENTICLE; CHAIN: B; | DNA (5'- CHAIN: C; DNA (5'- | CHAIN: D;                      | III.TRABITHORAX HOMEOTIC | PROTEIN IV; CHAIN: A; | HOMEOBOX PROTEIN      | EXTRADENTICLE; CHAIN: B; | DNA (5'- CHAIN: C; DNA (5'- | CHAIN: D;      | ENGRAIT ED HOMEODOMAIN: | Thomas and the second s |
| Table 5 | SEQ            | FOLD  |                    |                                             |                      |                                                        |                                          |                          |                               |                                              |                          |                               |                         |                      |                        |                       |                        |                          |                             |                                |                          |                       |                       |                          |                             |                |                         |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |
| Tat     | PMF            | score |                    | 0.52                                        |                      |                                                        |                                          | 98.0                     |                               |                                              | 0.77                     |                               |                         |                      | 9.65                   |                       |                        |                          |                             |                                | 0.84                     | 5                     |                       |                          |                             |                | 0.75                    | 55                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |
|         | Verify         | score |                    | 0.29                                        |                      |                                                        |                                          | 090                      |                               |                                              | 0.17                     |                               |                         |                      | 0.37                   |                       |                        |                          |                             |                                | 0.35                     | <br>                  |                       |                          |                             |                | 0.35                    | رن.۷                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |
|         | Psi            | Blast |                    | 6.8e-31                                     |                      |                                                        |                                          | 5 18-22                  |                               |                                              | 5.1e-25                  |                               |                         |                      | 3.4e-24                |                       |                        |                          |                             |                                | 3 AP-77                  | 7.75.6                |                       |                          |                             |                | 10.14                   | 12-14                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |
|         | END            | ΑĄ    |                    | 75                                          |                      |                                                        |                                          | 161                      | 1                             |                                              | 75                       | )<br>-                        |                         |                      | 159                    |                       |                        |                          |                             |                                | 73                       | C)                    |                       |                          |                             |                | 150                     | 100                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |
|         | START          | AA    |                    | 16                                          |                      |                                                        |                                          | 105                      | 2                             |                                              | 10                       | ;                             |                         |                      | 105                    |                       |                        |                          |                             |                                | 10                       | FT -                  |                       |                          |                             |                | 100                     | COT                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |
|         | CHAIN          | А     |                    | ď                                           |                      |                                                        |                                          | <                        | ς.                            |                                              | <b>V</b>                 | ď                             |                         |                      | A                      |                       |                        |                          |                             |                                |                          | ¥                     |                       |                          |                             |                | £                       | B                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |
|         | PDB            | A     |                    | 1ahd                                        |                      |                                                        |                                          | 11,77                    | 7/01                          |                                              | 1472                     | 7/01                          |                         |                      | 1b8i                   |                       |                        |                          |                             |                                | 11.0:                    | 1081                  |                       |                          |                             |                | -                       | 1 dag                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |
|         | SEO            | ́ДŞ́  | Ž                  | 1645                                        |                      |                                                        |                                          | 1645                     | 1040                          |                                              | 1645                     | 101                           |                         |                      | 1645                   |                       |                        |                          |                             |                                | 1745                     | 1045                  |                       |                          |                             |                |                         | 1645                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |

|         | PDB annotation | HAIN: C; HOMEOTIC PROTEIN ENGRAILED, SEGMENTATION POLARITY HOMEODOMAIN, DNABINDING PROTEIN, PROTEIN-DNA COMPLEX | N<br>OMAIN                                             | MAIN                                                   | IN: A, B,                                              |                                                     |                                                     | AIN: A, B, COMPLEX (DNA-BINDING |
|---------|----------------|-----------------------------------------------------------------------------------------------------------------|--------------------------------------------------------|--------------------------------------------------------|--------------------------------------------------------|-----------------------------------------------------|-----------------------------------------------------|---------------------------------|
|         | Compound       | CHAIN: A, B; DNA (5'- CHAIN: C;<br>DNA (5'- CHAIN: D;                                                           | DNA-BINDING PROTEIN<br>ENGRAILED HOMEODOMAIN<br>1ENH 3 | DNA-BINDING PROTEIN<br>ENGRAILED HOMEODOMAIN<br>1ENH 3 | PAIRED PROTEIN; CHAIN: A, B,<br>C; DNA; CHAIN: D, E, F | PAIRED PROTEIN; CHAIN: A, B, C; DNA; CHAIN: D, E, F | PAIRED PROTEIN; CHAIN: A, B, C; DNA; CHAIN: D, E, F | PAIRED PROTEIN; CHAIN: A, B,    |
| Table 5 | SEQ<br>FOLD    | 21000                                                                                                           |                                                        |                                                        |                                                        |                                                     |                                                     |                                 |
| Tal     | PMF<br>score   |                                                                                                                 | 0.95                                                   | 0.99                                                   | 0.92                                                   | 1.00                                                | 0.88                                                | 1.00                            |
|         | Verify         |                                                                                                                 | 0.39                                                   | 0.63                                                   | 0.28                                                   | 0.15                                                | 0.31                                                | 0.35                            |
|         | Psi<br>Blast   |                                                                                                                 | 6.8e-15                                                | 3.4e-19                                                | 3.4e-20                                                | 3.4e-25                                             | 3.4e-19                                             | 1.4e-23                         |
|         | END            |                                                                                                                 | 155                                                    | 69                                                     | 160                                                    | 74                                                  | 158                                                 | 72                              |
|         | START<br>AA    |                                                                                                                 | 103                                                    | 17                                                     | 102                                                    | 14                                                  | 102                                                 | 15                              |
|         | CHAIN          |                                                                                                                 |                                                        |                                                        | A                                                      | A                                                   | В                                                   | В                               |
|         | PDB            |                                                                                                                 | 1enh                                                   | 1enh                                                   | 141                                                    | 151                                                 | 161                                                 | 1fj1                            |
|         | SEQ            | Ö                                                                                                               | 1645                                                   | 1645                                                   | 1645                                                   | 1645                                                | 1645                                                | 1645                            |
|         |                |                                                                                                                 |                                                        |                                                        |                                                        |                                                     |                                                     |                                 |

| -        |                      |                                                                                            | —                                                                                |                                                                                  |                                                                                                                                                                             |                                                                                                                                                                             |                                                                                  |                                                         |
|----------|----------------------|--------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------|----------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------|---------------------------------------------------------|
|          | PDB annotation       | PROTEIN/DNA) DNA-<br>BINDING PROTEIN, DNA,<br>PAIRED BOX,<br>TRANSCRIPTION 2<br>REGULATION |                                                                                  |                                                                                  |                                                                                                                                                                             |                                                                                                                                                                             | COMPLEX (DNA BINDING PROTEIN/DNA) DNA BINDING, COMPLEX (DNA BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING PROTEIN/DNA) HD;                   |
|          | Compound             | C; DNA; CHAIN: D, E, F                                                                     | DNA-BINDING FUSHI TARAZU<br>PROTEIN (HOMEODOMAIN)<br>(NMR, 20 STRUCTURES) IFTZ 3 | DNA-BINDING FUSHI TARAZU<br>PROTEIN (HOMEODOMAIN)<br>(NMR, 20 STRUCTURES) 1FTZ 3 | DNA-BINDING PROTEIN ANTENNAPEDIA PROTEIN (HOMEODOMAIN) MUTANT WITH CYS 39 ISAN 3 REPLACED BY SER AND RESIDUES 1-6 DELETED (C39S,DEL 1-6) ISAN 4 (NMR, 20 STRUCTURES) ISAN 5 | DNA-BINDING PROTEIN ANTENNAPEDIA PROTEIN (HOMEODOMAIN) MUTANT WITH CYS 39 ISAN 3 REPLACED BY SER AND RESIDUES 1-6 DELETED (C39S,DEL 1-6) ISAN 4 (NMR, 20 STRUCTURES) ISAN 5 | ENGRAILED HOMEODOMAIN;<br>CHAIN: A, B; DNA (20-MER);<br>CHAIN: C, D;             | ANTENNAPEDIA PROTEIN;<br>CHAIN: A, B; DNA; CHAIN: C, D, |
| Table 5  | SEQ<br>FOLD<br>score |                                                                                            |                                                                                  |                                                                                  |                                                                                                                                                                             |                                                                                                                                                                             |                                                                                  |                                                         |
| <u>8</u> | PMF                  |                                                                                            | 0.46                                                                             | 0.01                                                                             | 0.72                                                                                                                                                                        | 0.78                                                                                                                                                                        | 0.92                                                                             | 99.0                                                    |
|          | Verify<br>score      |                                                                                            | 0.15                                                                             | -0.15                                                                            | 0.21                                                                                                                                                                        | 0.50                                                                                                                                                                        | 0.25                                                                             | 0.55                                                    |
|          | Psi<br>Blast         |                                                                                            | 8.5e-27                                                                          | 3.4e-23                                                                          | 5.1e-26                                                                                                                                                                     | 1.5e-28                                                                                                                                                                     | 3.4e-19                                                                          | 1.7e-25                                                 |
|          | END                  |                                                                                            | 82                                                                               | 166                                                                              | 166                                                                                                                                                                         | 75                                                                                                                                                                          | 71                                                                               | 160                                                     |
|          | START                |                                                                                            | 15                                                                               | 66                                                                               | 107                                                                                                                                                                         | 21                                                                                                                                                                          | 16                                                                               | 105                                                     |
|          | CHAIN                |                                                                                            |                                                                                  |                                                                                  |                                                                                                                                                                             |                                                                                                                                                                             | В                                                                                | A                                                       |
|          | PDB<br>ID            |                                                                                            | 1ftz                                                                             | 1ffz                                                                             | Isan                                                                                                                                                                        | lsan                                                                                                                                                                        | 2hdd                                                                             | 9ant                                                    |
|          | SEQ<br>ID            |                                                                                            | 1645                                                                             | 1645                                                                             | 1645                                                                                                                                                                        | 1645                                                                                                                                                                        | 1645                                                                             | 1645                                                    |

|         | PDB annotation |            | HOMEODOMAIN, COMPLEX<br>(DNA-BINDING<br>PROTEIN/DNA) | COMPLEX (DNA-BINDING PROTEIN/DNA) HD; HOMEODOMAIN, COMPLEX       | (DNA-BINDING<br>PROTEIN/DNA) | COMPLEX (BLOOD COAGULATION/INHIBITOR) AUTOPROTHROMBIN IIA;    | HYDROLASE, SERINE<br>PROTEINASE), PLASMA | CALCIUM BINDING, 2<br>GLYCOPROTEIN, COMPLEX | (BLOOD | COAGULATION/INHIBITOR) | HYDROLASE/HYDROLASE INHIBITOR PROTEIN-                  | PEPTIDE COMPLEX            |                             |                                            | SUGAR BINDING PROTEIN | UDA; LECTIN, HEVEIN        | SUPERANTIGEN | SUGAR BINDING PROTEIN | UDA; LECTIN, HEVEIN<br>DOMAIN, UDA,     |   |
|---------|----------------|------------|------------------------------------------------------|------------------------------------------------------------------|------------------------------|---------------------------------------------------------------|------------------------------------------|---------------------------------------------|--------|------------------------|---------------------------------------------------------|----------------------------|-----------------------------|--------------------------------------------|-----------------------|----------------------------|--------------|-----------------------|-----------------------------------------|---|
|         | Compound       |            | B, F,                                                | ANTENNAPEDIA PROTEIN;<br>CHAIN: A, B; DNA; CHAIN: C, D,<br>F. F: |                              | ACTIVATED PROTEIN C; CHAIN:<br>C, L; D-PHE-PRO-MAI; CHAIN: P; |                                          |                                             |        |                        | DES-GLA FACTOR VIIA (HEAVY CHAIN): CHAIN: H. I. DES-GLA | FACTOR VIIA (LIGHT CHAIN); | CHAIN: L, M; (DPN)-PHE-ARG; | CHAIN: C, D; PEPTIDE E-/6;<br>CHAIN: X, Y: | AGGLUTININ ISOLECTIN  | VI/AGGLUTININ ISOLECTIN V; | CHAIN: A;    | AGGI ITININ ISOLECTIN | VI/AGGLUTININ ISOLECTIN V;<br>CHAIN: A; |   |
| Table 5 | SEQ            | FOLD       |                                                      |                                                                  |                              | -                                                             |                                          |                                             |        |                        |                                                         | -                          |                             |                                            |                       |                            |              |                       |                                         | - |
| Tat     | PMF            | score      |                                                      | 0.78                                                             |                              | 0.33                                                          |                                          |                                             |        |                        | 0.19                                                    |                            | _                           |                                            | 0.11                  |                            |              | 0.07                  | <u> </u>                                |   |
|         | Verify         | score      |                                                      | 0.46                                                             |                              | 0.03                                                          |                                          |                                             |        |                        | -0.18                                                   |                            |                             |                                            | -0.02                 |                            |              | 0.15                  |                                         |   |
|         | Psi            | Blast      |                                                      | 5.1e-29                                                          |                              | 0.00024                                                       |                                          |                                             |        |                        | 9000.0                                                  |                            |                             |                                            | 7.2e-09               |                            |              | 60.05                 |                                         |   |
|         | END            | AA         |                                                      | 74                                                               |                              | 326                                                           |                                          |                                             |        |                        | 326                                                     |                            |                             |                                            | 200                   | ·<br>·                     |              | 07.0                  | 0/7                                     |   |
|         | START          | AA         |                                                      | 19                                                               |                              | 261                                                           |                                          |                                             |        |                        | 261                                                     |                            |                             |                                            | 115                   |                            |              | 707                   | 190                                     |   |
|         | CHAIN          | A          |                                                      | A                                                                |                              | 1                                                             | . 12-10                                  |                                             |        |                        | 1                                                       |                            |                             | •                                          | A                     | 4 7                        |              |                       | ∢                                       |   |
|         | PDB            | <u></u>    |                                                      | 9ant                                                             |                              | laut                                                          | - 7                                      |                                             | ····   |                        | 1dva                                                    |                            |                             |                                            | 1eic                  |                            |              |                       | leis                                    | _ |
|         | SEQ            | <br>百<br>矣 |                                                      | 1645                                                             |                              | 1646                                                          |                                          |                                             |        |                        | 1646                                                    |                            |                             |                                            | 1646                  | 2                          |              | ,                     | 1646                                    | _ |

|              |                |              |                                                                           | 2                                                                                                                                                                                   |                                                                            | ' | ای بر                                                                                       | ا م                                                                                         | _                                            |
|--------------|----------------|--------------|---------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------|---|---------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------|----------------------------------------------|
| הייויייי תחת | FDB annotation | SUPERANTIGEN | SIGNALLING PROTEIN<br>BINDING PROTEIN,<br>CYTOKINE, SIGNALLING<br>PROTEIN | COMPLEX (BLOOD COAGULATION/NHIBITOR) CHRISTMAS FACTOR; COMPLEX, INHIBITOR, HEMOPHILIA/EGF, BLOOD COAGULATION, 2 PLASMA, SERINE PROTEASE, CALCIUM-BINDING, HYDROLASE, 3 GLYCOPROTEIN | CONTRACTILE PROTEIN<br>TRIPLE-HELIX COILED<br>COIL, CONTRACTILE<br>PROTEIN |   | DNA-BINDING HMGA DNA-<br>BINDING HMG-BOX<br>DOMAIN A OF RAT HMG1;<br>1AAB 8 HMG-BOX 1AAB 20 | DNA-BINDING HMGA DNA-<br>BINDING HMG-BOX<br>DOMAIN A OF RAT HMG1;<br>1AAB 8 HMG-BOX 1AAB 20 | DNA BINDING PROTEIN<br>HMG BOX, DNA BENDING, |
|              | Compound       |              | TUMOR NECROSIS FACTOR<br>RECEPTOR; CHAIN: A, B;                           | FACTOR IXA; CHAIN: C, L,; D-<br>PHE-PRO-ARG; CHAIN: I;                                                                                                                              | HUMAN SKELETAL MUSCLE<br>ALPHA-ACTININ 2; CHAIN: A;                        |   | HIGH MOBILITY GROUP<br>PROTEIN; 1AAB 5 CHAIN: NULL;<br>1AAB 6                               | HIGH MOBILITY GROUP<br>PROTEIN; 1AAB 5 CHAIN: NULL;<br>1AAB 6                               | NON HISTONE PROTEIN 6 A;<br>CHAIN: A;        |
| Table 5      | SEQ<br>FOLD    |              | 63.01                                                                     | 64.18                                                                                                                                                                               |                                                                            |   |                                                                                             |                                                                                             | 51.42                                        |
| Tat          | PMF            |              |                                                                           |                                                                                                                                                                                     | -0.20                                                                      |   | 0.39                                                                                        | 0.54                                                                                        |                                              |
|              | Verify score   |              |                                                                           |                                                                                                                                                                                     | 0.08                                                                       |   | 0.61                                                                                        | -0.00                                                                                       |                                              |
| i            | Psi<br>Blast   |              | 2.4e-14                                                                   | 2.4e-13                                                                                                                                                                             | 90-99                                                                      |   | 2.4e-16                                                                                     | 1.7e-09                                                                                     | 3.4e-12                                      |
|              | END            |              | 249                                                                       | 144                                                                                                                                                                                 | 148                                                                        |   | 173                                                                                         | 151                                                                                         | 172                                          |
|              | START<br>AA    |              | 86                                                                        | 10                                                                                                                                                                                  | 21                                                                         |   | 93                                                                                          | 94                                                                                          | 80                                           |
|              | CHAIN          |              | A                                                                         | 1                                                                                                                                                                                   | A                                                                          |   |                                                                                             |                                                                                             | A                                            |
|              | PDB<br>ID      | -            | lext                                                                      | 1pfx                                                                                                                                                                                | 1quu                                                                       |   | 1aab                                                                                        | 1aab                                                                                        | 1cg7                                         |
|              | SEQ            | :<br>S       | 1646                                                                      | 1646                                                                                                                                                                                | 1647                                                                       |   | 1649                                                                                        | 1649                                                                                        | 1649                                         |

|         | PDB annotation |          | DNA RECOGNITION,<br>CHROMATIN, NMR, DNA 2<br>BINDING PROTEIN | DNA BINDING PROTEIN<br>HMG BOX, DNA BENDING,<br>DNA RECOGNITION, | CHROMATIN, NMR, DNA 2<br>BINDING PROTEIN | GENE REGULATION/DNA<br>HMG-1, AMPHOTERIN,            | HEPARIN-BINDING PROTEIN B20: HIGH MORIT ITY | GROUP DOMAIN, BENT | DNA, PROTEIN-DRUG-DNA 2<br>COMPLEX, GENE | REGULATION/DNA |                           |                          |                         |                          |                           |                          |                            |                         |                          |        |                                                    |                            |
|---------|----------------|----------|--------------------------------------------------------------|------------------------------------------------------------------|------------------------------------------|------------------------------------------------------|---------------------------------------------|--------------------|------------------------------------------|----------------|---------------------------|--------------------------|-------------------------|--------------------------|---------------------------|--------------------------|----------------------------|-------------------------|--------------------------|--------|----------------------------------------------------|----------------------------|
|         | Compound       |          |                                                              | NON HISTONE PROTEIN 6 A;<br>CHAIN: A;                            |                                          | HIGH MOBILITY GROUP 1<br>PROTEIN; CHAIN: A; DNA (5'- | D(*CP*CP*(IDO) CHAIN: B; DNA                | (5'- CHAIN: C;     |                                          |                | DNA-BINDING HIGH MOBILITY | GROUP PROTEIN FRAGMENT-B | HMG-BOX DOMAIN B OF RAT | HMG1) (NMR, 1 STRUCTURE) | DNA-BINDING HIGH MOBILITY | GROUP PROTEIN FRAGMENT-B | (HMGB) (DNA-BINDING 1HME 3 | HMG-BOX DOMAIN B OF RAT | HMG1) (NMR, 1 STRUCTURE) | IHME 4 | DNA-BINDING HIGH MOBILITY GROUP PROTEIN FRAGMENT-B | (HMGB) (DNA-BINDING 1HME 3 |
| Table 5 | SEQ<br>FOI D   | score    |                                                              |                                                                  |                                          |                                                      |                                             |                    |                                          |                | 51.33                     |                          |                         |                          |                           |                          |                            |                         |                          |        |                                                    |                            |
| Tak     | PMF            | aloos    |                                                              | 0.81                                                             |                                          | -0.08                                                |                                             |                    |                                          |                |                           |                          |                         |                          | 0.18                      |                          |                            |                         |                          |        | 0.87                                               |                            |
|         | Verify         | score    |                                                              | -0.05                                                            |                                          | 0.25                                                 |                                             |                    |                                          |                |                           |                          |                         |                          | 0.41                      |                          |                            |                         |                          |        | 0.12                                               |                            |
|         | Psi            | Blast    |                                                              | 3.4e-12                                                          |                                          | 6e-14                                                |                                             |                    |                                          |                | 1.1e-12                   |                          |                         | _                        | 3.4e-09                   |                          |                            |                         |                          |        | 1.1e-12                                            |                            |
|         | END            | AA       |                                                              | 152                                                              |                                          | 173                                                  |                                             |                    |                                          |                | 170                       |                          |                         |                          | 177                       |                          |                            |                         |                          |        | 148                                                |                            |
|         | START          | AA       |                                                              | 85                                                               |                                          | 100                                                  |                                             |                    |                                          |                | 95                        | 1                        |                         |                          | 95                        | )                        |                            |                         |                          |        | 76                                                 |                            |
|         | CHAIN          | <br>A    |                                                              | A                                                                |                                          | A                                                    |                                             |                    |                                          |                |                           |                          |                         |                          |                           |                          |                            |                         |                          |        |                                                    |                            |
|         | PDB            | ——<br>А  |                                                              | 1cg7                                                             |                                          | 1ckt                                                 |                                             |                    |                                          |                | 1hme                      |                          |                         |                          | 11-me                     | 211111                   |                            |                         |                          |        | 1hme                                               |                            |
|         | SEQ            | <u> </u> | 2                                                            | 1649                                                             |                                          | 1649                                                 |                                             |                    |                                          |                | 1649                      |                          |                         |                          | 1640                      | 10+7                     |                            |                         |                          |        | 1649                                               |                            |

| Ģ.      | PDB annotation  |                                                               |                                                                                                                                                        |                                                                                                                                                        |                                                                                                                                                        | GENE REGULATION/DNA HMG-D; PROTEIN-DNA COMPLEX, HMG DOMAIN, NON-SEQUENCE SPECIFIC 2 CHROMOSOMAL PROTEIN HMG-D        | GENE REGULATION/DNA<br>HMG-D; PROTEIN-DNA<br>COMPLEX, HMG DOMAIN,<br>NON-SEQUENCE SPECIFIC 2         |
|---------|-----------------|---------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------|
|         | Compound        | HMG-BOX DOMAIN B OF RAT<br>HMG1) (NMR, 1 STRUCTURE)<br>1HME 4 | DNA-BINDING HIGH MOBILITY<br>GROUP PROTEIN 1 (HMG1) BOX<br>2, COMPLEXED WITH 1HSM 3<br>MERCAPTOETHANOL (NMR,<br>MINIMIZED AVERAGE<br>STRUCTURE) 1HSM 4 | DNA-BINDING HIGH MOBILITY<br>GROUP PROTEIN 1 (HMG1) BOX<br>2, COMPLEXED WITH 1HSM 3<br>MERCAPTOETHANOL (NMR,<br>MINIMIZED AVERAGE<br>STRUCTURE) 1HSM 4 | DNA-BINDING HIGH MOBILITY<br>GROUP PROTEIN 1 (HMG1) BOX<br>2, COMPLEXED WITH 1HSM 3<br>MERCAPTOETHANOL (NMR,<br>MINIMIZED AVERAGE<br>STRUCTURE) 1HSM 4 | DNA (5'-<br>D(*GP*CP*GP*AP*TP*AP*TP*CP<br>*GP*C)-3'); CHAIN: C, D; HIGH<br>MOBILITY GROUP PROTEIN D;<br>CHAIN: A, B; | DNA (5'-<br>D(*GP*CP*GP*AP*TP*AP*TP*CP<br>*GP*C)-3'); CHAIN: C, D; HIGH<br>MOBILITY GROUP PROTEIN D; |
| Table 5 | SEQ<br>FOLD     | score                                                         |                                                                                                                                                        |                                                                                                                                                        |                                                                                                                                                        |                                                                                                                      |                                                                                                      |
| Lab     | PMF<br>score    |                                                               | 0.89                                                                                                                                                   | 0.01                                                                                                                                                   | 0.24                                                                                                                                                   | 0.21                                                                                                                 | 0.63                                                                                                 |
|         | Verify<br>score |                                                               | 0.22                                                                                                                                                   | -0.06                                                                                                                                                  | -0.10                                                                                                                                                  | 0.31                                                                                                                 | 0.29                                                                                                 |
|         | Psi<br>Blast    |                                                               | 1.2e-11                                                                                                                                                | 1.2e-12                                                                                                                                                | 1.7e-08                                                                                                                                                | 2.4e-10                                                                                                              | 1.7e-07                                                                                              |
|         | END<br>AA       |                                                               | 148                                                                                                                                                    | 295                                                                                                                                                    | 179                                                                                                                                                    | 141                                                                                                                  | 168                                                                                                  |
|         | START           |                                                               | 100                                                                                                                                                    | 220                                                                                                                                                    | 86                                                                                                                                                     | 100                                                                                                                  | 86                                                                                                   |
|         | CHAIN           |                                                               |                                                                                                                                                        |                                                                                                                                                        |                                                                                                                                                        | A                                                                                                                    | A                                                                                                    |
|         | PDB             |                                                               | 1hsm                                                                                                                                                   | 1hsm                                                                                                                                                   | 1hsm                                                                                                                                                   | 1qrv                                                                                                                 | lqrv                                                                                                 |
|         | SEQ             | NO:                                                           | 1649                                                                                                                                                   | 1649                                                                                                                                                   | 1649                                                                                                                                                   | 1649                                                                                                                 | 1649                                                                                                 |

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|---------|----------------|------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------|-------------------------|
|         | PDB annotation | CHROMOSOMAL PROTEIN<br>HMG-D | GENE REGULATION/DNA LEF-1 HMG; LEF1, HMG, TCR-A, TRANSCRIPTION FACTOR, DNA BINDING, DNA 2 BENDING, COMPLEX (HMG DOMAIN/DNA), GENE REGULATION/DNA | COMPLEX (ZINC<br>FINGER/DNA) COMPLEX<br>(ZINC FINGER/DNA), ZINC<br>FINGER, DNA-BINDING         | COMPLEX (ZINC<br>FINGER/DNA) COMPLEX<br>(ZINC FINGER/DNA), ZINC<br>FINGER, DNA-BINDING<br>PROTEIN | COMPLEX (ZINC<br>FINGER/DNA) COMPLEX<br>(ZINC FINGER/DNA), ZINC<br>FINGER, DNA-BINDING<br>PROTEIN | COMPLEX (ZINC<br>FINGER/DNA) COMPLEX<br>(ZINC FINGER/DNA), ZINC<br>FINGER, DNA-BINDING<br>PROTEIN | COMPLEX (ZINC           |
|         | Compound       | CHAIN: A, B;                 | LYMPHOID ENHANCER-<br>BINDING FACTOR; CHAIN: A;<br>DNA (5'- CHAIN: B; DNA (5'-<br>CHAIN: C;                                                      | QGSR ZINC FINGER PEPTIDE;<br>CHAIN: A; DUPLEX<br>OLIGONUCLEOTIDE BINDING<br>SITE; CHAIN: B, C; | QGSR ZINC FINGER PEPTIDE;<br>CHAIN: A; DUPLEX<br>OLIGONUCLEOTIDE BINDING<br>SITE; CHAIN: B, C;    | QGSR ZINC FINGER PEPTIDE;<br>CHAIN: A; DUPLEX<br>OLIGONUCLEOTIDE BINDING<br>SITE; CHAIN: B, C;    | QGSR ZINC FINGER PEPTIDE;<br>CHAIN: A; DUPLEX<br>OLIGONUCLEOTIDE BINDING<br>SITE; CHAIN: B, C;    | DNA; CHAIN: A, B, D, E; |
| Table 5 | SEQ<br>FOLD    | SCOLE                        |                                                                                                                                                  |                                                                                                | 73.66                                                                                             |                                                                                                   |                                                                                                   | 83.90                   |
| Tab     | PMF<br>score   |                              | 0.47                                                                                                                                             | 1.00                                                                                           |                                                                                                   | 0.00                                                                                              | -0.01                                                                                             |                         |
|         | Verify score   |                              | 0.15                                                                                                                                             | 0.30                                                                                           |                                                                                                   | -0.11                                                                                             | 0.01                                                                                              |                         |
|         | Psi<br>Blast   |                              | 2.4e-15                                                                                                                                          | 1.5e-30                                                                                        | 1.6e-34                                                                                           | 3.4e-21                                                                                           | 5.1e-25                                                                                           | 5.1e-51                 |
|         | END            |                              | 179                                                                                                                                              | 274                                                                                            | 276                                                                                               | 151                                                                                               | 171                                                                                               | 274                     |
|         | START<br>AA    |                              | 101                                                                                                                                              | 194                                                                                            | 194                                                                                               | 63                                                                                                | 66                                                                                                | 193                     |
|         | CHAIN          |                              | A                                                                                                                                                | A                                                                                              | A                                                                                                 | A                                                                                                 | А                                                                                                 | C                       |
|         | PDB<br>ID      |                              | 21ef                                                                                                                                             | 1a1h                                                                                           | lalh                                                                                              | la1h                                                                                              | lalh                                                                                              | 1mey                    |
|         | SEQ<br>ID      | NO.                          | 1649                                                                                                                                             | 1651                                                                                           | 1651                                                                                              | 1651                                                                                              | 1651                                                                                              | 1651                    |

|         | PDB annotation  | FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC<br>FINGER/DNA) ZINC FINGER,<br>PROTEIN-DNA<br>INTERACTION, PROTEIN<br>DESIGN, 2 CRYSTAL<br>STRUCTURE, COMPLEX<br>(ZINC FINGER/DNA) | COMPLEX (ZINC<br>FINGER/DNA) ZINC FINGER,<br>PROTEIN-DNA<br>INTERACTION, PROTEIN<br>DESIGN, 2 CRYSTAL<br>STRUCTURE, COMPLEX<br>(ZINC FINGER/DNA) | COMPLEX (TRANSCRIPTION REGULATION/DNA) COMPLEX (TRANSCRIPTION REGULATION/DNA), RNA POLYMERASE III, 2 TRANSCRIPTION INITIATION, ZINC FINGER PROTEIN | COMPLEX (TRANSCRIPTION<br>REGULATION/DNA) YING-<br>YANG 1; TRANSCRIPTION |
|---------|-----------------|------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------|
|         | Compound        | CONSENSUS ZINC FINGER<br>PROTEIN; CHAIN: C, F, G;                                                                | DNA; CHAIN: A, B, D, E;<br>CONSENSUS ZINC FINGER<br>PROTEIN; CHAIN: C, F, G;                                                                     | DNA; CHAIN: A, B, D, E;<br>CONSENSUS ZINC FINGER<br>PROTEIN; CHAIN: C, F, G;                                                                     | TFIIIA; CHAIN: A, D; 5S<br>RIBOSOMAL RNA GENE; CHAIN:<br>B, C, E, F;                                                                               | YYI; CHAIN: C; ADENO-<br>ASSOCIATED VIRUS P5<br>INITIATOR ELEMENT DNA;   |
| Table 5 | SEQ<br>FOLD     |                                                                                                                  |                                                                                                                                                  |                                                                                                                                                  | 67.48                                                                                                                                              | 71.38                                                                    |
| Tat     | PMF             |                                                                                                                  | 1.00                                                                                                                                             | 0.07                                                                                                                                             |                                                                                                                                                    |                                                                          |
|         | Verify<br>score |                                                                                                                  | 0.43                                                                                                                                             | 0.17                                                                                                                                             |                                                                                                                                                    |                                                                          |
|         | Psi<br>Blast    |                                                                                                                  | 5.1e-51                                                                                                                                          | 3.4e-40                                                                                                                                          | 4e-34                                                                                                                                              | 1.8e-34                                                                  |
|         | END             |                                                                                                                  | 274                                                                                                                                              | 151                                                                                                                                              | 274                                                                                                                                                | 274                                                                      |
|         | START           |                                                                                                                  | 193                                                                                                                                              | 62                                                                                                                                               | 66                                                                                                                                                 | 166                                                                      |
|         | CHAIN           |                                                                                                                  | U                                                                                                                                                | U                                                                                                                                                | Ą                                                                                                                                                  | O                                                                        |
|         | PDB<br>ID       |                                                                                                                  | 1mey                                                                                                                                             | lmey                                                                                                                                             | 1116                                                                                                                                               | 1ubd                                                                     |
|         | SEQ             | <br>OZ                                                                                                           | 1651                                                                                                                                             | 1651                                                                                                                                             | 1651                                                                                                                                               | 1651                                                                     |

|         | PDB annotation |       | INITIATION, INITIATOR<br>ELEMENT, YY1, ZINC 2<br>FINGER PROTEIN, DNA- | PROTEIN RECOGNITION, 3 | COMPLEX (TRANSCRIPTION<br>REGULATION/DNA) | COMPLEX (DNA-BINDING      | FINGER GLI; GLI, ZINC       | FINGER, COMPLEX (DNA- | NO FROI ELIVIDINE) | SERINE ESTERASE<br>HYDROLASE, SERINE | ESTERASE, GLYCOPROTEIN | SERINE ESTERASE        | HYDROLASE, SEKINE<br>ESTERASE, GLYCOPROTEIN | SERINE ESTERASE        | HYDROLASE, SERINE<br>ESTERASE, GI VCOPROTEIN | TRANSFERASE | DINUCLEOTIDE-BINDING       | MOTIF, PHOSPHORIBOSYL<br>TRANSFERASE | TRANSFERASE | DINUCLEOTIDE-BINDING       | MOTIF, PHOSPHORIBOSYL<br>TRANSFERASE | HYDROLASE               | NEURAMINIDASE; |
|---------|----------------|-------|-----------------------------------------------------------------------|------------------------|-------------------------------------------|---------------------------|-----------------------------|-----------------------|--------------------|--------------------------------------|------------------------|------------------------|---------------------------------------------|------------------------|----------------------------------------------|-------------|----------------------------|--------------------------------------|-------------|----------------------------|--------------------------------------|-------------------------|----------------|
|         |                |       | INITIA'<br>ELEME<br>FINGEI                                            | PROTE                  | COMPI                                     | COMPI                     | FINGE                       | FINGE                 | חאוום              | SERIN                                | ESTER                  | SERIN                  | HYDR                                        | SERIN                  | HYDR                                         | TRAN        | DINIO                      | MOTI                                 | TRAN        | DINIC                      | MOTI                                 | HYDR                    | NEUR           |
|         | Compound       |       | CHAIN: A, B;                                                          |                        |                                           | ZINC FINGER PROTEIN GLII; | CHAIN: A; DNA; CHAIN: C, D; |                       |                    | CUTINASE; CHAIN: NULL;               |                        | CUTINASE; CHAIN: NULL; |                                             | CUTINASE; CHAIN: NULL; |                                              | NICOTINATE  | MONONUCLEOTIDE:5,6- CHAIN: | A;                                   | NICOTINATE  | MONONUCLEOTIDE:5,6- CHAIN: | A;                                   | SIALIDASE; CHAIN: NULL; |                |
| Table 5 | SEQ<br>FOLD    | score |                                                                       |                        |                                           | 82.80                     |                             |                       |                    |                                      |                        |                        |                                             |                        |                                              |             |                            |                                      |             |                            |                                      |                         |                |
| Tal     | PMF            |       |                                                                       |                        |                                           |                           |                             |                       |                    | -0.14                                |                        | -0.17                  |                                             | -0.15                  |                                              | 0.10        | .;<br>                     |                                      |             | -0.19                      |                                      | -0.17                   |                |
|         | Verify         |       |                                                                       |                        |                                           |                           |                             |                       |                    | 0.59                                 |                        | 0.21                   |                                             | 0.70                   |                                              | 0.10        | 0.13                       |                                      | 0           | 0.77                       |                                      | 0.20                    |                |
|         | Psi<br>Blast   | 15117 |                                                                       | _                      |                                           | 1.6e-38                   |                             |                       |                    | 2.4e-11                              |                        | 3.6e-08                |                                             | 1.2e-10                |                                              | 100 15      | 4.05-1.7                   |                                      | 9           | 7.2e-42                    |                                      | 1.2e-08                 |                |
|         | END            | V.    |                                                                       |                        |                                           | 277                       |                             |                       |                    | 307                                  |                        | 201                    |                                             | 290                    | )<br>\<br>\                                  | 173         | 7/1                        |                                      | 0,0         | 363                        |                                      | 306                     |                |
|         | START          | ξ     |                                                                       |                        |                                           | 126                       |                             |                       |                    | 132                                  |                        | 48                     |                                             | 64                     | -<br>                                        | 5           | ¢7                         |                                      |             | 34                         |                                      | 175                     |                |
|         | CHAIN          | 3     |                                                                       |                        |                                           | A                         |                             |                       |                    |                                      |                        |                        | 112                                         |                        |                                              |             | <b>Y</b>                   |                                      |             | ¥.                         |                                      |                         |                |
|         | PDB            |       |                                                                       |                        |                                           | 2gli                      |                             |                       |                    | 1cex                                 |                        | 1cex                   |                                             | 1.                     | V T                                          | ,           | sop I                      |                                      |             | 140s                       |                                      | 1011                    | Tent           |
|         | SEQ            | <br>∃ |                                                                       |                        |                                           | 1651                      |                             |                       |                    | 1660                                 |                        | 1660                   |                                             | 1660                   | 7001                                         |             | 1660                       |                                      |             | 1660                       |                                      | 1660                    | 1000           |

|         | PDB annotation |          | HYDROLASE,<br>GLYCOSIDASE | HYDROLASE               | NEURAMINIDASE; | HYDROLASE,<br>GI VCOSIDASE | TD ANSEED ASE AT DHA- | SUPERHELIX,             | TRANSFERASE |                                          | MEMBRANE PROTEIN VSG | VSG, TRYPANOSOME,        | ANTIGENIC VARIATION, | MEMBRANE PROTEIN | HYDROLASE UREA              | AMINOHYDROLASE; UREA        | AMINOHYDROLASE; UREA        | AMINOHYDROLASE; | UREASE, BACILLUS | PASTEURII, NICKEL, | ACETOHYDROXAMIC ACID, | 2 METALLOGING IME | THE STATE OF THE TOTAL THE | PHYDROLASE CZ DOMAJIN, | PHOSPHOTASE                        | HYDROLASE | HYDDOI ACE DITAI       | SPECIFICITY         | PHOSPHATASE, MAP |  |
|---------|----------------|----------|---------------------------|-------------------------|----------------|----------------------------|-----------------------|-------------------------|-------------|------------------------------------------|----------------------|--------------------------|----------------------|------------------|-----------------------------|-----------------------------|-----------------------------|-----------------|------------------|--------------------|-----------------------|-------------------|----------------------------|------------------------|------------------------------------|-----------|------------------------|---------------------|------------------|--|
|         | Compound       |          |                           | SIALIDASE: CHAIN: NULL; |                |                            | Correct Bilymic       | TRANSGLYCOSYLASE SLT70; | CHAIN: A;   | VIRUS TOMATO BUSHY STUNT<br>VIRUS 2TBV 4 | VARIANT SURFACE      | GLYCOPROTEIN ILTAT 1.24; | CHAIN: A, B;         |                  | UREASE (CHAIN A); CHAIN: A; | UREASE (CHAIN B); CHAIN: B; | UREASE (CHAIN C); CHAIN: C; |                 |                  |                    |                       |                   |                            | PHOSPHOINOSITIDE       | IIIOSI IIO IASE I LEIV, CIELLIIII, |           | PATORIA OTTA DE ATILET | FYS11; CHAIN: NOLL; |                  |  |
| Table 5 | SEQ            | score    |                           |                         |                |                            |                       |                         |             |                                          |                      |                          |                      |                  |                             |                             |                             |                 |                  |                    |                       |                   |                            |                        |                                    |           |                        |                     |                  |  |
| Tał     | PMF            | Score    |                           | -0.18                   | :              |                            | :                     | 0.11                    |             | -0.19                                    | -0.19                |                          |                      |                  | -0.19                       |                             |                             |                 |                  |                    |                       |                   |                            | 0.57                   |                                    |           |                        | 0.49                |                  |  |
|         | Verify         | score    |                           | 0 19                    | 3              |                            |                       | -0.10                   |             | 0.22                                     | 0.09                 |                          |                      |                  | 0.09                        |                             |                             |                 |                  |                    |                       |                   |                            | 0.26                   |                                    |           |                        | 0.10                |                  |  |
|         | Psi            | Blast    |                           | 4 RP-00                 | )<br>)<br>)    |                            |                       | 7.2e-05                 |             | 8.4e-09                                  | 4.8e-12              |                          |                      |                  | 4.8e-19                     |                             |                             |                 |                  |                    |                       |                   |                            | 8.5e-17                |                                    |           |                        | 3.4e-16             |                  |  |
|         | END:           | AA       |                           | 307                     | 775            |                            |                       | 196                     |             | 412                                      | 411                  | !<br>!                   |                      |                  | 445                         |                             |                             |                 |                  |                    |                       |                   |                            | 137                    |                                    |           |                        | 139                 |                  |  |
|         | START          | AA       |                           | 230                     | 007            |                            |                       | 873                     |             | 139                                      | 133                  | )                        |                      |                  | 32                          |                             |                             |                 |                  |                    |                       |                   |                            | 9                      |                                    |           |                        | 9                   |                  |  |
|         | CHAIN          | <br>A    |                           |                         |                |                            |                       | Ą                       |             | C                                        | <b>V</b>             | <b>1.7</b>               |                      |                  | C                           | )                           |                             |                 |                  |                    |                       |                   |                            | A                      |                                    |           |                        |                     |                  |  |
|         | PDB            | <br>A    |                           | 1011                    | l eni          |                            |                       | 1qsa                    |             | 2tbv                                     | 2,700                | 5°17                     | -                    |                  | 4ubn                        | ).<br>}                     |                             |                 |                  |                    |                       |                   |                            | 1d5r                   |                                    |           |                        | 1mkp                |                  |  |
|         | SEQ            | —<br>A Ş | į                         | 1660                    | 1000           |                            |                       | 1660                    |             | 1660                                     | 1660                 | 7001                     |                      |                  | 1660                        | 2                           |                             |                 |                  |                    |                       |                   |                            | 1668                   |                                    |           |                        | 1668                |                  |  |

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|         | PDB amotation | KINASE HYDROLASE | COMPLEX (GTP-BINDING/EFFECTOR) RAS-RELATED PROTEIN RAB3A; COMPLEX (GTP-BINDING/EFFECTOR), GPROTEIN, EFFECTOR, RABCDR, 2 SYNAPTIC EXOCYTOSIS, RABPROTEIN, RAB3A, | RABPHILIN COMPLEX (GTP- BINDING/EFFECTOR) RAS- RELATED PROTEIN RAB3A; COMPLEX (GTP- BINDING/EFFECTOR), G PROTEIN, EFFECTOR, RABCDR, 2 SYNAPTIC EXOCYTOSIS, RAB PROTEIN, RAB3A, RABPHILIN | HYDROLASE INHIBITOR<br>ALL-BETA STRUCTURE,<br>HYDROLASE INHIBITOR | HYDROLASE INHIBITOR<br>ALL-BETA STRUCTURE,<br>HYDROLASE INHIBITOR | SERINE PROTEINASE<br>COAGULATION FACTOR II;          |
|---------|---------------|------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------|-------------------------------------------------------------------|------------------------------------------------------|
|         | Compound      |                  | RAB-3A; CHAIN: A; RABPHILIN-3A; CHAIN: B;                                                                                                                       | RAB-3A; CHAIN: A; RABPHILIN-3A; CHAIN: B;                                                                                                                                                | BOWMAN-BIRK TRYPSIN<br>INHIBITOR; CHAIN: A                        | BOWMAN-BIRK TRYPSIN<br>INHIBITOR; CHAIN: A                        | THROMBIN LIGHT CHAIN;<br>CHAIN: A, B, C, D; THROMBIN |
| Table 5 | SEQ<br>FOLD   |                  |                                                                                                                                                                 |                                                                                                                                                                                          |                                                                   |                                                                   |                                                      |
| Tab     | PMF           |                  | 0.37                                                                                                                                                            | 0.15                                                                                                                                                                                     | -0.18                                                             | -0.18                                                             | -0.12                                                |
|         | Verify        |                  | 0.07                                                                                                                                                            | 0.29                                                                                                                                                                                     | 0.89                                                              | 0.89                                                              | 0.99                                                 |
|         | Psi<br>Blast  |                  | 0.004                                                                                                                                                           | 0.00085                                                                                                                                                                                  | 9.6e-15                                                           | 9.6e-15                                                           | 6e-11                                                |
|         | END           |                  | 367                                                                                                                                                             | 358                                                                                                                                                                                      | 103                                                               | 103                                                               | 103                                                  |
|         | START<br>AA   |                  | 311                                                                                                                                                             | 313                                                                                                                                                                                      | 3                                                                 | 3                                                                 | 4                                                    |
|         | CHAIN<br>ID   |                  | В                                                                                                                                                               | В                                                                                                                                                                                        | A                                                                 | A                                                                 | I                                                    |
|         | PDB<br>ID     |                  | 1zbd                                                                                                                                                            | 1zbd                                                                                                                                                                                     | 1c2a                                                              | 1c2a                                                              | 1dx5                                                 |
|         | SHQ<br>US:    | 5 .              | 1674                                                                                                                                                            | 1674                                                                                                                                                                                     | 1704                                                              | 1704                                                              | 1704                                                 |

|         | PDB annotation |       | COAGULATION FACTOR II;<br>FETOMODULIN, TM, CD141<br>ANTIGEN; EGR-CMK SERINE           | PROTEINASE, EGF-LIKE         | DOMESTICO AGULANT | COMPLEX, 2 | ANTIFIBRINOLY IIC<br>COMPLEX | SERINE PROTEINASE     | COAGULATION FACTOR II;       | FETOMODULIN, TM, CD141    | ANTIGEN; EGR-CMK SERINE        | PROTEINASE, EGF-LIKE         | DOMENINS, | AN IICOAGOLAINI | COMPLEA, 2 | AN ILFIBRATION INC. COMPLEX | SUGAR BINDING PROTEIN | UDA; LECTIN, HEVEIN        | DOMAIN, UDA, | SUPERANTIGEN | SUGAR BINDING PROTEIN | UDA; LECTIN, HEVEIN        | DOMAIN, UDA, | SUPERANTIGEN | SUGAR BINDING PROTEIN | DOMAIN, UDA, |
|---------|----------------|-------|---------------------------------------------------------------------------------------|------------------------------|-------------------|------------|------------------------------|-----------------------|------------------------------|---------------------------|--------------------------------|------------------------------|-----------|-----------------|------------|-----------------------------|-----------------------|----------------------------|--------------|--------------|-----------------------|----------------------------|--------------|--------------|-----------------------|--------------|
|         | Compound       |       | HEAVY CHAIN; CHAIN: M, N, O, P; THROMBOMODULIN; CHAIN: I, J, K, L; THROMBIN INHIBITOR | L-GLU-L-GLY-L-ARM; CHAIN: E, | г, С, н;          |            |                              | THROMBIN LIGHT CHAIN; | HEAVY CHAIN: CHAIN: M. N. O. | P; THROMBOMODULIN; CHAIN: | I, J, K, L; THROMBIN INHIBITOR | L-GLU-L-GLY-L-AKM; CHAIN: E, | r, c, मु; |                 |            |                             | AGGLUTININ ISOLECTIN  | VI/AGGLUTININ ISOLECTIN V; | CHAIN: A;    |              | AGGLUTININ ISOLECTIN  | VI/AGGLUTININ ISOLECTIN V; | CHAIN: A;    |              | AGGLUTININ ISOLECTIN  | CHAIN: A;    |
| Table 5 | SEQ<br>FOI D   | score |                                                                                       |                              |                   |            |                              |                       |                              |                           |                                |                              |           |                 |            |                             |                       |                            |              |              |                       |                            |              |              |                       |              |
| Tal     | PMF            | 21026 |                                                                                       |                              |                   |            |                              | -0.12                 |                              |                           |                                |                              |           |                 |            |                             | 0.04                  |                            |              |              | 0.04                  |                            |              |              | -0.08                 |              |
|         | Verify         | SCOTO |                                                                                       |                              |                   |            |                              | 0.99                  |                              |                           |                                |                              |           |                 |            |                             | 1.29                  |                            |              |              | 1.29                  |                            |              |              | 0.91                  |              |
|         | Psi            | Didst |                                                                                       |                              |                   |            |                              | 6e-11                 |                              |                           |                                | •                            |           |                 |            |                             | 4.8e-13               |                            |              |              | 4.8e-13               |                            |              |              | 1.2e-17               |              |
|         | END            | £     |                                                                                       |                              |                   |            |                              | 103                   |                              |                           | -                              |                              |           |                 |            |                             | 62                    |                            |              |              | 62                    |                            |              |              | 101                   |              |
|         | START          | ¥     |                                                                                       |                              |                   |            |                              | 4                     |                              |                           |                                |                              |           |                 |            |                             | 1                     |                            |              |              | 1                     |                            |              |              | 9                     |              |
|         | CHAIN          |       |                                                                                       |                              |                   | _          |                              |                       |                              |                           |                                |                              | -         |                 |            |                             | A                     |                            |              |              | A                     |                            |              |              | A                     |              |
|         | PDB            |       |                                                                                       |                              |                   |            |                              | 1dx5                  |                              |                           |                                |                              |           |                 |            |                             | 1eis                  | }                          |              |              | 1eis                  |                            |              |              | 1eis                  |              |
|         | SEQ            | a ġ   |                                                                                       |                              |                   |            |                              | 1704                  |                              |                           |                                |                              |           |                 |            |                             | 1704                  |                            |              |              | 1704                  |                            |              |              | 1704                  |              |

|         | PDB annotation |          | SUPERANTIGEN | SUGAR BINDING PROTEIN<br>UDA; LECTIN, HEVEIN       | DOMAIN, UDA,<br>SUPERANTIGEN | SIGNALLING PROTEIN    | BINDING PROTEIN,<br>CYTOKINE, SIGNALLING | PROTEIN | SIGNALLING PROTEIN    | BINDING FROIEST,       | PROTEIN | EXTRACELLULAR MODULE | OSTEONECTIN, SPARC,         | SECKETED PROTEIN ACIDIC | AND EXTRACELLULAR | MODULE, GLYCOPROTEIN, | AN II-ADHESIVE FROIEIN, 2 | COLLAGEN BINDING, SITE- | DIKECLED MOTAGENESIS, | GLYCOSYLATED 3 PROTEIN | MODKES | EXTRACELLULAR MODULE | OSTEONECTIN, SPARC,         | SECKETED PROTEIN ACIDIC | AND EXTRACELLULAR | MODULE, GLYCOPROTEIN, | ANTI-ADHESIVE PROTEIN, 2 | DIRECTED MUTAGENESIS, |  |
|---------|----------------|----------|--------------|----------------------------------------------------|------------------------------|-----------------------|------------------------------------------|---------|-----------------------|------------------------|---------|----------------------|-----------------------------|-------------------------|-------------------|-----------------------|---------------------------|-------------------------|-----------------------|------------------------|--------|----------------------|-----------------------------|-------------------------|-------------------|-----------------------|--------------------------|-----------------------|--|
|         | Compound       |          |              | AGGLUTININ ISOLECTIN<br>VI/AGGLUTININ ISOLECTIN V. | CHAIN: A;                    | TUMOR NECROSIS FACTOR | RECEPTOR; CHAIN: A, B;                   |         | TUMOR NECROSIS FACTOR | RECEPTOR; CHAIN: A, B; |         | BASEMENT MEMBRANE    | PROTEIN BM-40; CHAIN: A, B; |                         |                   |                       |                           |                         |                       |                        |        | BASEMENT MEMBRANE    | PROTEIN BM-40; CHAIN: A, B; |                         |                   |                       |                          |                       |  |
| Table 5 | SEQ            | FOLD     | -            |                                                    |                              |                       |                                          |         |                       |                        |         |                      |                             |                         |                   |                       |                           |                         |                       |                        |        |                      | •••                         |                         |                   |                       |                          |                       |  |
| Tal     | PMF            | score    |              | -0.08                                              |                              | -0.13                 |                                          |         | -0.13                 |                        |         | -0.19                |                             |                         |                   |                       |                           |                         |                       |                        |        | -0.19                |                             |                         |                   |                       |                          |                       |  |
|         | Verify         | score    |              | 0.91                                               |                              | 0.51                  |                                          |         | 0.51                  |                        |         | 0.57                 |                             |                         |                   |                       |                           |                         |                       |                        |        | 0.57                 |                             |                         |                   |                       |                          |                       |  |
|         | Psi            | Blast    |              | 1.2e-17                                            |                              | 1 28-00               | 27:1                                     |         | 1.2e-09               |                        |         | 3.6e-16              |                             |                         |                   |                       |                           |                         |                       |                        |        | 3.6e-16              |                             |                         |                   |                       |                          |                       |  |
|         | END            | AA       |              | 101                                                |                              | 103                   | 3                                        |         | 103                   |                        |         | 102                  | l<br>                       |                         |                   |                       |                           |                         |                       |                        |        | 102                  |                             |                         |                   |                       |                          |                       |  |
|         | START          | AA       |              | 9                                                  |                              | ,                     | ٧                                        |         | 2                     |                        |         | ~                    | 1                           | ·-                      |                   |                       |                           |                         |                       |                        |        | 3                    | ı                           |                         |                   |                       |                          |                       |  |
|         | CHAIN          | А        |              | A                                                  |                              |                       | τ                                        |         | A                     |                        |         | A                    | 4 7                         |                         |                   |                       |                           |                         |                       |                        |        | A                    | 4                           |                         |                   |                       |                          |                       |  |
|         | PDB            | <u></u>  |              | 1eis                                               |                              | 1                     | ובאו                                     |         | lext                  |                        |         | 1mih                 | Onni                        |                         |                   |                       |                           |                         |                       |                        |        | Inih                 |                             |                         |                   |                       | -4-                      |                       |  |
|         | SEQ            | <u> </u> |              | 1704                                               |                              | 1707                  | 1/04                                     |         | 1704                  |                        |         | 1704                 | 10/1                        |                         |                   |                       |                           |                         |                       |                        |        | 1704                 | 5                           |                         |                   |                       |                          |                       |  |

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|         |                |          |                               |                              |                        |                   |                     |                       |                        |                  |                  |              |              |                              |                        |                   |                     |                       |                        |                  |                  |              |              |                          |                 |                |                    |               | _                     |                  | $\overline{}$ |                          |      |
|---------|----------------|----------|-------------------------------|------------------------------|------------------------|-------------------|---------------------|-----------------------|------------------------|------------------|------------------|--------------|--------------|------------------------------|------------------------|-------------------|---------------------|-----------------------|------------------------|------------------|------------------|--------------|--------------|--------------------------|-----------------|----------------|--------------------|---------------|-----------------------|------------------|---------------|--------------------------|------|
| 1 1 1   | PDB annotation |          | GLYCOSYLATED 3 PROTEIN MODRES | COMPLEX (BLOOD               | COAGULATION/INHIBITOR) | CHRISTMAS FACTOR; | COMPLEX, INHIBITOR, | HEMOPHILIA/EGF, BLOOD | COAGULATION, 2 PLASMA, | SERINE PROTEASE, | CALCIUM-BINDING, | HYDROLASE, 3 | GLYCOPROTEIN | COMPLEX (BLOOD               | COAGULATION/INHIBITOR) | CHRISTMAS FACTOR; | COMPLEX, INHIBITOR, | HEMOPHILIA/EGF, BLOOD | COAGULATION, 2 PLASMA, | SERINE PROTEASE, | CALCIUM-BINDING, | HYDROLASE, 3 | GLYCOPROTEIN | MEMBRANE ADHESION        | SHORT CONSENSUS | REPEAT, SUSHI, | COMPLEMENT CONTROL | PROTEIN, 2 N- | GLYCOSYLATION, MULTI- | DOMAIN, MEMBRANE | ADHESION      | MEMBRANE ADHESION        |      |
|         | Compound       |          |                               | FACTOR IXA; CHAIN: C, L.; D- | PHE-PRO-ARG; CHAIN: I; |                   |                     |                       |                        |                  |                  |              |              | FACTOR IXA: CHAIN: C. L.; D- | PHE_DRO_ARG: CHAIN: I: | TIME TIME (TIME)  |                     |                       |                        |                  |                  |              |              | HUMAN BETAZ-GLYCOPROTEIN | I: CHAIN: A:    |                |                    |               |                       |                  |               | HUMAN BETA2-GLYCOPROTEIN |      |
| Table 5 | SEQ            | FOLD     |                               |                              |                        |                   |                     |                       |                        |                  |                  |              |              |                              |                        |                   |                     |                       |                        |                  |                  |              |              |                          |                 |                |                    |               |                       |                  |               |                          |      |
| Tal     | PMF            | score    |                               | -0.12                        | !                      |                   |                     |                       |                        |                  |                  |              |              | -0.12                        | 71.0                   |                   |                     |                       |                        |                  |                  |              |              | -0 19                    | }               |                |                    |               |                       |                  |               | -0.19                    |      |
|         | Verify         | score    |                               | 98 0                         | ?                      |                   |                     |                       |                        |                  |                  |              |              | 920                          | 00.0                   |                   |                     |                       | ·                      |                  |                  |              |              | 0 07                     | }               |                |                    |               |                       |                  |               | 0.97                     |      |
|         | Psi            | Blast    |                               | 1 20-11                      | 11.77:1                |                   |                     |                       |                        |                  |                  |              |              | 1 20 11                      | 1.22-11                |                   |                     |                       |                        |                  |                  |              |              | 8 4P-16                  | 01-21-0         |                |                    |               |                       |                  |               | 8 4e-16                  | 21.0 |
|         | END            | AA       |                               | 103                          | 201                    |                   |                     |                       |                        |                  |                  |              |              | 102                          | co1                    |                   |                     |                       |                        |                  |                  |              |              | 103                      | 5               |                |                    |               |                       |                  |               | 103                      | 100  |
|         | START          | AA       |                               | 16                           | 91                     |                   |                     |                       |                        |                  |                  |              |              | 1                            | 10                     |                   |                     |                       |                        |                  |                  |              |              | ,                        | 7               |                |                    |               |                       |                  |               | ,                        | 7    |
|         | CHAIN          |          |                               | 1                            | <u> </u>               |                   |                     |                       |                        |                  |                  |              |              |                              |                        |                   |                     |                       |                        |                  |                  |              |              |                          | ₹.              |                |                    |               |                       |                  |               |                          | 4    |
|         | PDB            | <u>a</u> | +                             |                              | - XIďI                 |                   |                     |                       | -                      |                  |                  |              |              | ,                            | Iptx                   |                   |                     |                       |                        |                  |                  |              |              |                          | anbı            |                |                    |               |                       |                  |               | 1.5                      | onbi |
|         | SEQ            | Э        | S                             | 700                          | 1/04                   |                   |                     |                       |                        |                  |                  |              | _            |                              | 1704                   |                   |                     |                       |                        |                  |                  |              |              | ,000                     | 1/04            |                |                    |               |                       |                  |               | 7 7 7                    | 1/04 |

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| Table 5 | SEQ    |
| Tal     | PMF    |
|         | Verify |
|         | Psi    |
|         | END    |

| Г       |                      |                                                                          | Т                                                     | T                                                              |                                                                | <br>                |                                                    |                     |                                                    |                     |                                                    |                     |                           | Т                     |                                           | <u> </u>              |                                            |
|---------|----------------------|--------------------------------------------------------------------------|-------------------------------------------------------|----------------------------------------------------------------|----------------------------------------------------------------|---------------------|----------------------------------------------------|---------------------|----------------------------------------------------|---------------------|----------------------------------------------------|---------------------|---------------------------|-----------------------|-------------------------------------------|-----------------------|--------------------------------------------|
|         | PDB annotation       | SHORT CONSENSUS<br>REPEAT, SUSHI,<br>COMPLEMENT CONTROL<br>PROTEIN, 2 N- | GLYCOSYLATION, MULTI-<br>DOMAIN, MEMBRANE<br>ADHESION | PLASMINOGEN<br>ACTIVATION                                      | PLASMINOGEN<br>ACTIVATION                                      | GLYCOSIDASE CGTASE; | 1CIU 8 THERMOSTABLE<br>1CIU 14                     | GLYCOSIDASE CGTASE; | 1CIU 8 THERMOSTABLE                                | GLYCOSIDASE CGTASE; | 1CIU 8 THERMOSTABLE<br>1CIU 14                     | GLYCOSIDASE CGTASE; | 1CIU 8 THERMOSTABLE       | CI VCOSIDA SE CGTASE: | ICIU 8 THERMOSTABLE                       | 1CIU 14               | GLYCOSIDASE CGTASE;<br>1CIU 8 THERMOSTABLE |
|         | Compound             | I; CHAIN: A;                                                             |                                                       | T-PLASMINOGEN ACTIVATOR<br>F1-G; 1TPG 7 CHAIN: NULL;<br>1TPG 8 | T-PLASMINOGEN ACTIVATOR<br>F1-G; 1TPG 7 CHAIN: NULL;<br>1TPG 8 | CYCLODEXTRIN        | GLYCOSYLTRANSFERASE; 1CIU<br>6 CHAIN: NULL; 1CIU 7 | CYCLODEXTRIN        | GLYCOSYLTRANSFERASE; 1CIU<br>6 CHAIN: NULL; 1CIU 7 | CYCLODEXTRIN        | GLYCOSYLTRANSFERASE; 1CIU<br>6 CHAIN: NULL; 1CIU 7 | CYCLODEXTRIN        | GLYCOSYLTRANSFERASE; 1CIU | 6 CHAIN: NOLL; ICIU / | CYCLODEXIKUN<br>GLYCOSYLTRANSFERASE; 1CIU | 6 CHAIN: NULL; 1CIU 7 | CYCLODEXTRIN<br>GLYCOSYLTRANSFERASE; 1CIU  |
| Table 5 | SEQ<br>FOLD<br>score |                                                                          |                                                       |                                                                |                                                                |                     |                                                    |                     |                                                    |                     |                                                    |                     |                           |                       |                                           |                       |                                            |
| Tab     | PMF<br>score         |                                                                          |                                                       | 0.04                                                           | 0.04                                                           | -0.19               |                                                    | -0.19               |                                                    | -0.19               |                                                    | -0.20               |                           |                       | -0.20                                     |                       | -0.20                                      |
|         | Verify<br>score      |                                                                          |                                                       | 1.31                                                           | 1.31                                                           | 0.18                |                                                    | 0.00                | )<br>)                                             | 0.15                |                                                    | 0.20                |                           |                       | 0.02                                      |                       | 0.02                                       |
|         | Psi<br>Blast         |                                                                          |                                                       | 3.6e-07                                                        | 3.6e-07                                                        | 7.2e-22             |                                                    | 2 4P-25             | 2                                                  | 3.6e-26             |                                                    | 2 4e-25             | 3                         |                       | 4.8e-25                                   |                       | 2.4e-26                                    |
|         | END                  |                                                                          |                                                       | 91                                                             | 91                                                             | 1309                |                                                    | 1485                |                                                    | 1570                | )                                                  | 1677                |                           |                       | 1736                                      |                       | 1792                                       |
|         | START<br>AA          |                                                                          |                                                       | 4                                                              | 4                                                              | 1025                |                                                    | 1150                | 0011                                               | 1204                |                                                    | 13.48               | 2                         |                       | 1380                                      |                       | 1429                                       |
|         | CHAIN                |                                                                          |                                                       |                                                                |                                                                |                     |                                                    |                     |                                                    |                     |                                                    |                     |                           |                       |                                           |                       |                                            |
|         | PDB<br>ID            |                                                                          |                                                       | 1tpg                                                           | 1tpg                                                           | 1cin                | 5                                                  | 10ii                | ıcın                                               | 13.                 |                                                    | 10::                | 1010                      |                       | 1ciu                                      |                       | 1ciu                                       |
|         | SEQ<br>ID            |                                                                          |                                                       | 1704                                                           | 1704                                                           | 1706                |                                                    | 1705                | 1/00                                               | 1706                |                                                    | 1706                | 0/1                       |                       | 1706                                      |                       | 1706                                       |

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|----------|----------------|----------|-----------------------|--------------------------------------------|-----------------------|---------------------|----------------------------------------------------|---------------------|---------------------------|-----------------------|----------------------|---------------------------|-----------------------|---------------------|---------------------------|-----------------------|---------------------|---------------------------|-----------------------|---------------------|---------------------------|-----------------------|---------------------|---------------------------|-----------------------|---------------------|---------------------------|-----------------------|---------------------|--------------|--------------------|
|          | PDB annotation |          | 1CIU 14               | GLYCOSIDASE CGTASE;<br>ICIU 8 THERMOSTABLE | 1CIU 14               | GLYCOSIDASE CGTASE; | ICIU 8 THERMOSTABLE<br>ICIU 14                     | GLYCOSIDASE CGTASE; | 1CIU 8 THERMOSTABLE       | ICIU 14               | GLYCOSIDASE CGITASE; | ICIU 8 THERMOSTABLE       | ICIU 14               | GLYCOSIDASE CGTASE; | 1CIU 8 THERMOSTABLE       | 1CIU 14               | GLYCOSIDASE CGTASE; | 1CIU 8 THERMOSTABLE       | 1CIU 14               | GLYCOSIDASE CGTASE; | 1CIU 8 THERMOSTABLE       | 1CIU 14               | GLYCOSIDASE CGTASE; | 1CIU 8 THERMOSTABLE       | 1CIU 14               | GLYCOSIDASE CGTASE; | 1CIU 8 THERMOSTABLE       | 1CIU 14               |                     |              |                    |
|          | Compound       |          | 6 CHAIN: NULL; 1CIU 7 | CYCLODEXTRIN<br>GLYCOSYLTRANSFERASE; 1CIU  | 6 CHAIN: NULL; 1CIU 7 | CYCLODEXTRIN        | GLYCOSYLTRANSFERASE; 1CIU<br>6 CHAIN: NULL; 1CIU 7 | CYCLODEXTRIN        | GLYCOSYLTRANSFERASE; 1CIU | 6 CHAIN: NULL; 1CIU 7 | CYCLODEXTRIN         | GLYCOSYLTRANSFERASE; 1CIU | 6 CHAIN: NULL; 1CIU 7 | CYCLODEXTRIN        | GLYCOSYLTRANSFERASE; 1CIU | 6 CHAIN: NULL; 1CIU 7 | CYCLODEXTRIN        | GLYCOSYLTRANSFERASE; 1CIU | 6 CHAIN: NULL; 1CIU 7 | CYCLODEXTRIN        | GLYCOSYLTRANSFERASE; 1CIU | 6 CHAIN: NULL; 1CIU 7 | CYCLODEXTRIN        | GLYCOSYLTRANSFERASE; 1CIU | 6 CHAIN: NULL; 1CIU 7 | CYCLODEXTRIN        | GLYCOSYLTRANSFERASE; 1CIU | 6 CHAIN: NULL; 1CIU 7 | GLYCOSYLTRANSFERASE | CYCLODEXIKIN | GLUCANOIRANSFERASE |
| I able 5 | SEQ            | FOLD     |                       |                                            |                       |                     |                                                    |                     |                           |                       |                      |                           |                       |                     |                           |                       |                     |                           |                       |                     |                           |                       |                     |                           |                       |                     |                           |                       |                     |              |                    |
| Jac      | PMF            | score    |                       | -0.19                                      |                       | -0.18               |                                                    | -0.19               |                           |                       | -0.18                |                           |                       | -0.20               |                           |                       | -0.20               |                           |                       | -0.20               |                           |                       | -0.20               |                           |                       | -0.20               |                           |                       | -0.19               |              |                    |
|          | Verify         | score    |                       | 0.03                                       |                       | 90.0                |                                                    | 0.03                |                           |                       | 0.13                 |                           |                       | 0.12                |                           |                       | 0.16                |                           |                       | 0.19                |                           |                       | 60.0                |                           |                       | 0.01                |                           |                       | 0.01                |              |                    |
|          | Psi            | Blast    |                       | 1.1e-22                                    |                       | 2.4e-24             |                                                    | 2.4e-21             |                           |                       | 8.4e-27              |                           |                       | 9.6e-28             |                           |                       | 8.4e-27             |                           |                       | 6e-28               |                           |                       | 3.6e-26             |                           |                       | 7.2e-22             |                           |                       | 7.2e-32             |              |                    |
|          | END            | AA       |                       | 1824                                       |                       | 1915                |                                                    | 1933                |                           |                       | 21.9                 |                           |                       | 746                 |                           |                       | 778                 | •                         |                       | 886                 |                           |                       | 965                 |                           |                       | 1060                | 2                         |                       | 1533                |              |                    |
|          | START          | AA       |                       | 1492                                       |                       | 1572                |                                                    | 1633                |                           |                       | 315                  |                           |                       | 408                 | )                         |                       | 469                 | )<br>)                    |                       | 552                 |                           |                       | 601                 |                           |                       | 757                 | 2                         |                       | 1091                |              |                    |
|          | CHAIN          | <u> </u> |                       |                                            |                       |                     |                                                    |                     |                           |                       |                      |                           |                       |                     |                           |                       |                     |                           |                       |                     |                           |                       |                     |                           |                       |                     |                           |                       |                     |              |                    |
|          | PDB            | А        |                       | 1ciu                                       |                       | 1ciu                |                                                    | 1cin                | 101                       |                       | 1ciu                 |                           |                       | 1cin                | 3                         |                       | 1ciii               | 101                       |                       | 1,cin               | 1                         |                       | 1cin                |                           |                       | 1cin                | 1                         |                       | 1cyg                |              |                    |
|          | SEQ            | ΒŞ       |                       | 1706                                       |                       | 1706                |                                                    | 1706                | 2                         |                       | 1706                 | )                         |                       | 1706                | 2                         |                       | 1706                | 2007                      |                       | 1706                | 200                       |                       | 1706                | 2                         |                       | 1706                | 00/1                      |                       | 1706                |              |                    |

| -       |                | - $-$    |                                |                     |              |                    | $\neg$                         |                     |              | _                  | $\neg$                         |                     | _            |                    |                                |                     |              |                    | —T                             |                     |              |                    |                                |                     |              |                    | ļ                             |                     |              |                    | Į.                             |                     | - 1          |
|---------|----------------|----------|--------------------------------|---------------------|--------------|--------------------|--------------------------------|---------------------|--------------|--------------------|--------------------------------|---------------------|--------------|--------------------|--------------------------------|---------------------|--------------|--------------------|--------------------------------|---------------------|--------------|--------------------|--------------------------------|---------------------|--------------|--------------------|-------------------------------|---------------------|--------------|--------------------|--------------------------------|---------------------|--------------|
|         | PDB annotation |          |                                |                     |              |                    |                                |                     |              |                    |                                |                     |              |                    |                                |                     |              |                    |                                |                     |              |                    |                                |                     |              |                    |                               |                     |              |                    |                                |                     |              |
|         | Compound       |          | (E.C.2.4.1.19) (CGTASE) 1CYG 3 | GLYCOSYLTRANSFERASE | CYCLODEXTRIN | GLUCANOTRANSFERASE | (E.C.2.4.1.19) (CGTASE) 1CYG 3 | GLYCOSYLTRANSFERASE | CYCLODEXTRIN | GLUCANOTRANSFERASE | (E.C.2.4.1.19) (CGTASE) 1CYG 3 | GLYCOSYLTRANSFERASE | CYCLODEXTRIN | GLUCANOTRANSFERASE | (E.C.2.4.1.19) (CGTASE) 1CYG 3 | GLYCOSYLTRANSFERASE | CYCLODEXTRIN | GLUCANOTRANSFERASE | (E.C.2.4.1.19) (CGTASE) 1CYG 3 | GLYCOSYLTRANSFERASE | CYCLODEXTRIN | GLUCANOTRANSFERASE | (E.C.2.4.1.19) (CGTASE) 1CYG 3 | GLYCOSYLTRANSFERASE | CYCLODEXTRIN | GLUCANOTRANSFERASE | (E.C.2.4.1.19) (CGTASE) 1CYG3 | GLYCOSYLTRANSFERASE | CYCLODEXTRIN | GLUCANOTRANSFERASE | (E.C.2.4.1.19) (CGTASE) 1CYG 3 | GLYCOSYLTRANSFERASE | CYCLODEXTRIN |
| Table 5 | SEQ            | FOLD     |                                |                     |              |                    |                                |                     |              |                    |                                |                     |              |                    |                                |                     |              |                    |                                |                     |              |                    |                                |                     |              |                    |                               |                     |              |                    |                                |                     |              |
| Tat     | PMF            | score    |                                | -0.19               |              |                    |                                | -0.19               |              |                    |                                | -0.20               |              |                    |                                | -0.20               |              |                    |                                | -0.20               |              |                    |                                | -0.19               |              |                    |                               | -0.19               |              |                    |                                | -0.19               |              |
|         | Verify         | score    |                                | 0.07                |              |                    |                                | 0.15                |              |                    |                                | 0.01                |              |                    |                                | 90.0                |              |                    |                                | 0.17                |              |                    |                                | 0.20                |              |                    |                               | 0.10                |              |                    |                                | 0.14                |              |
|         | Psi            | Blast    |                                | 1.2e-30             |              |                    |                                | 6e-28               |              |                    |                                | 1.2e-27             |              |                    |                                | 3.6e-29             |              |                    |                                | 8.4e-31             |              |                    |                                | 2.4e-32             |              |                    |                               | 4.8e-31             |              |                    |                                | 1.1e-26             |              |
|         | END            | AA       |                                | 1677                |              |                    |                                | 1840                |              |                    |                                | 1920                |              |                    |                                | 548                 | !            |                    |                                | 858                 |              |                    |                                | 884                 |              |                    |                               | 196                 | ·            |                    |                                | 1206                | 1            |
|         | START          | AA       |                                | 1241                |              |                    |                                | 1420                |              |                    |                                | 1485                |              |                    |                                | 186                 | )            |                    |                                | 420                 |              |                    |                                | 495                 |              |                    |                               | 544                 |              |                    |                                | 752                 |              |
|         | CHAIN          | <u> </u> |                                |                     |              |                    |                                |                     |              |                    |                                |                     |              |                    |                                |                     |              |                    |                                |                     |              |                    |                                |                     |              |                    |                               |                     |              |                    |                                |                     |              |
|         | PDB            | <u> </u> |                                | lcvg                | 0            |                    |                                | 1cvg                |              |                    |                                | 1000                | D (2)        |                    |                                | 1000                | 1038         |                    | -                              | 1cvo                | a Ca         |                    |                                | 1cvo                | 200          |                    |                               | 1 cva               | 1078         |                    |                                | 1cva                | 3621         |
|         | SEQ            | ΑŞ       |                                | 1706                |              |                    |                                | 1706                |              |                    |                                | 1706                | 2            |                    |                                | 1706                | 20/1         |                    |                                | 1706                | 3            |                    |                                | 1706                |              |                    |                               | 1706                | 8            |                    |                                | 1706                | 3            |

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|         | PDB annotation       |                                                      |                                     |                                                      |                                                      |                                                         | HYDROLASE BETA-ALPHA<br>(TIM) BARREL | HYDROLASE               | NEURAMINIDASE; | GLYCOSIDASE, | HYDROLASE               | NEURAMINIDASE; | HYDROLASE,<br>GLYCOSIDASE | HYDROL ASE                   | NEURAMINIDASE; | HYDROLASE, | HYDROI ASE                | NEURAMINIDASE;           | HYDROLASE, | GLYCOSIDASE | HYDROLASE NET ID A MINIDA SE | HYDROLASE, |  |
|---------|----------------------|------------------------------------------------------|-------------------------------------|------------------------------------------------------|------------------------------------------------------|---------------------------------------------------------|--------------------------------------|-------------------------|----------------|--------------|-------------------------|----------------|---------------------------|------------------------------|----------------|------------|---------------------------|--------------------------|------------|-------------|------------------------------|------------|--|
|         | Compound             | GLUCANOTRANSFERASE<br>(E.C.2.4.1.19) (CGTASE) 1CYG 3 | GLYCOSYLTRANSFERASE<br>CYCLODEXTRIN | GLUCANOTRANSFERASE<br>(E.C.2.4.1.19) (CGTASE) 1CYG 3 | CATALYTIC ANTIBODY 17E8<br>COMPLEXED WITH PHENYL [1- | (1-N-SUCCINYLAMINO)PENTYL]<br>1EAP 3 PHOSPHONATE 1EAP 4 | CHITINASE A; CHAIN: A;               | SIALIDASE; CHAIN: NULL; |                |              | SIALIDASE; CHAIN: NULL; |                |                           | STAT IDASE: CHAIN: NI II I : |                |            | SIAT TO SE. CHAIN: NITITE | SINDIANE, CITAIN: NO.EE, |            |             | SIALIDASE; CHAIN: NULL;      |            |  |
| Table 5 | SEQ<br>FOLD<br>score |                                                      |                                     |                                                      |                                                      |                                                         |                                      |                         |                |              |                         |                |                           |                              |                |            |                           |                          |            |             |                              |            |  |
| Ta      | PMF                  |                                                      | -0.20                               |                                                      | 0.18                                                 |                                                         | 0.07                                 | -0.19                   |                |              | -0.19                   |                |                           | 010                          | 9<br>          |            | 0                         | -0.10                    |            |             | -0.19                        |            |  |
|         | Verify<br>score      |                                                      | 0.18                                |                                                      | 0.21                                                 |                                                         | -0.17                                | 90.0                    |                |              | 0.05                    |                |                           | 200                          | co.o           |            | 0,0                       | 0.30                     |            |             | 0.12                         |            |  |
|         | Psi<br>Blast         |                                                      | 2.4e-29                             |                                                      | 0.0024                                               |                                                         | 0.00012                              | 2.4e-18                 |                |              | 2.4e-17                 |                |                           | 1.0                          | 1.26-19        |            | 0                         | 27-90°C                  |            |             | 8.4e-20                      |            |  |
|         | END                  |                                                      | 1293                                | -                                                    | 1791                                                 |                                                         | 1290                                 | 1345                    |                |              | 1455                    | 2              |                           | 1000                         | C0C1           |            | Į.                        | /101/                    |            |             | 1677                         |            |  |
|         | START<br>AA          |                                                      | 838                                 |                                                      | 1707                                                 |                                                         | 1203                                 | 1103                    |                |              | 1210                    | 2121           |                           |                              | 1313           | •          |                           | 1389                     |            |             | 1437                         |            |  |
|         | CHAIN                |                                                      |                                     |                                                      | В                                                    |                                                         | A                                    |                         |                |              |                         |                |                           |                              |                |            |                           |                          |            |             |                              |            |  |
|         | PDB<br>ID            |                                                      | lcyg                                |                                                      | leap                                                 |                                                         | ledq                                 | 1eut                    |                |              | 1ent                    | i ca           |                           |                              | leut           |            |                           | l leut                   |            |             | leut                         |            |  |
|         | SEQ<br>ID<br>NO:     |                                                      | 1706                                |                                                      | 1706                                                 |                                                         | 1706                                 | 1706                    | )              |              | 1706                    | 0/1            |                           |                              | 1706           |            |                           | 1706                     |            |             | 1706                         |            |  |

| le 5    |  |
|---------|--|
| Table : |  |
|         |  |
|         |  |
|         |  |

|         | PDB annotation |         | GLYCOSIDASE | HYDROLASE<br>NEURAMINIDASE: | HYDROLASE, | GLYCOSIDASE | HYDROLASE               | NEURAMINIDASE;    | HYDROLASE, | OLI COSIDASE | HYDROLASE               | NEURAMINIDASE; | HYDROLASE, | GLYCOSIDASE | HYDROLASE               | NEURAMINIDASE; | HYDROLASE, | GLYCOSIDASE | CHAPERONE/STRUCTURAL<br>PROTEIN CHAPERONE                   | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
|         | Compound       |         |             | SIALIDASE; CHAIN: NULL;     |            |             | SIALIDASE; CHAIN: NULL; |                   |            |              | SIALIDASE; CHAIN: NULL; |                |            |             | SIALIDASE; CHAIN: NULL; |                |            |             | PAPD-LIKE CHAPERONE FIMC;<br>CHAIN: A, C, E, G, I, K, M, O; |
| Table 5 | SEQ            | score   |             |                             |            |             |                         |                |            |             |                         |                |            |             |                         |                |            |             |                         |                   |            |              |                         |                |            |             |                         |                |            |             |                                                             |
| Tab     | PMF            | score   |             | -0.17                       |            |             | -0.20                   |                | , ***      |             | -0.17                   |                |            |             | -0.20                   |                |            |             | -0.15                   |                   |            |              | -0.18                   |                |            |             | -0.20                   |                |            |             | -0.17                                                       |
|         | Verify         | score   |             | 0.18                        |            |             | 0.08                    |                |            |             | 0.08                    |                |            |             | 80.0                    |                |            |             | 0.10                    |                   |            |              | -0.00                   |                |            |             | 0.02                    |                |            |             | 0.01                                                        |
|         | Psi            | Blast   |             | 1.2e-19                     |            |             | 9.6e-15                 |                |            |             | 2.4e-22                 | _              |            |             | 2.4e-20                 |                |            |             | 1.2e-16                 |                   |            |              | 6e-17                   |                |            |             | 2.4e-16                 |                |            |             | 2.4e-35                                                     |
|         | END:           | AA      |             | 1835                        |            |             | 1933                    |                |            |             | 789                     |                |            |             | 098                     |                |            |             | 1217                    |                   |            |              | 1289                    |                |            |             | 1309                    |                |            |             | 1521                                                        |
|         | START          | AA      |             | 1514                        |            |             | 1658                    | )<br>)<br>)    |            |             | 462                     | <u> </u>       |            |             | 609                     |                |            |             | 989                     | 2                 |            |              | 926                     |                |            |             | 686                     |                |            |             | 1255                                                        |
|         | CHAIN          | A       |             |                             |            |             |                         |                |            |             |                         |                |            |             |                         |                |            |             |                         |                   |            |              |                         |                |            |             |                         |                |            |             | В                                                           |
|         | PDB            | ——<br>白 |             | 1eut                        |            |             | 1ent                    | 17.7           |            |             | 1ent                    |                |            |             | 1eut                    |                |            |             | 1 trial                 | זה היותר<br>היותר |            |              | 1eut                    | •              |            |             | 1eut                    |                |            |             | 1qun                                                        |
|         | SEQ            | e Š     |             | 1706                        |            |             | 1706                    | 2              |            |             | 1706                    | 8              |            |             | 1706                    | ;              |            |             | 1706                    | 8                 |            |              | 1706                    |                |            |             | 1706                    |                |            |             | 1706                                                        |

|         | PDB annotation       | ADHESIN DONOR STRAND<br>COMPLEMENTATION, 2<br>CHAPERONE/STRUCTURAL<br>PROTEIN | CHAPERONE/STRUCTURAL PROTEIN CHAPERONE ADHESIN DONOR STRAND COMPLEMENTATION, 2 CHAPERONE/STRUCTURAL PROTEIN                        | CHAPERONE/STRUCTURAL PROTEIN CHAPERONE ADHESIN DONOR STRAND COMPLEMENTATION, 2 CHAPERONE/STRUCTURAL PROTEIN                        | CHAPERONE/STRUCTURAL PROTEIN CHAPERONE ADHESIN DONOR STRAND COMPLEMENTATION, 2 CHAPERONE/STRUCTURAL PROTEIN                        | CHAPERONE/STRUCTURAI<br>PROTEIN CHAPERONE<br>ADHESIN DONOR STRAND<br>COMPLEMENTATION, 2<br>CHAPERONE/STRUCTURAI<br>PROTEIN         | CHAPERONE/STRUCTURAI<br>PROTEIN CHAPERONE<br>ADHESIN DONOR STRAND                       |
|---------|----------------------|-------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------|
|         | Compound             | MANNOSE-SPECIFIC ADHESIN<br>FIMH; CHAIN: B, D, F, H, J, L, N,<br>P;           | PAPD-LIKE CHAPERONE FIMC;<br>CHAIN: A, C, E, G, I, K, M, O;<br>MANNOSE-SPECIFIC ADHESIN<br>FIMH; CHAIN: B, D, F, H, J, L, N,<br>P; | PAPD-LIKE CHAPERONE FIMC;<br>CHAIN: A, C, E, G, I, K, M, O;<br>MANNOSE-SPECIFIC ADHESIN<br>FIMH; CHAIN: B, D, F, H, J, L, N,<br>P; | PAPD-LIKE CHAPERONE FIMC;<br>CHAIN: A, C, E, G, I, K, M, O;<br>MANNOSE-SPECIFIC ADHESIN<br>FIMH; CHAIN: B, D, F, H, J, L, N,<br>P; | PAPD-LIKE CHAPERONE FIMC;<br>CHAIN: A, C, E, G, I, K, M, O;<br>MANNOSE-SPECIFIC ADHESIN<br>FIMH; CHAIN: B, D, F, H, J, L, N,<br>P; | PAPD-LIKE CHAPERONE FIMC,<br>CHAIN: A, C, E, G, I, K, M, O;<br>MANNOSE-SPECIFIC ADHESIN |
| Table 5 | SEQ<br>FOLD<br>score |                                                                               |                                                                                                                                    |                                                                                                                                    |                                                                                                                                    |                                                                                                                                    |                                                                                         |
| Ta      | PMF                  |                                                                               | -0.19                                                                                                                              | -0.20                                                                                                                              | -0.19                                                                                                                              | -0.19                                                                                                                              | -0.20                                                                                   |
|         | Verify               |                                                                               | 0.09                                                                                                                               | 0.16                                                                                                                               | 0.19                                                                                                                               | 0.29                                                                                                                               | 0.13                                                                                    |
|         | Psi<br>Blast         |                                                                               | 9.6e-37                                                                                                                            | 1.1e-35                                                                                                                            | 3.6e-34                                                                                                                            | 8.4e-32                                                                                                                            | 1.2e-34                                                                                 |
|         | END                  |                                                                               | 1613                                                                                                                               | 1697                                                                                                                               | 1745                                                                                                                               | 1808                                                                                                                               | 645                                                                                     |
|         | START                |                                                                               | 1338                                                                                                                               | 1402                                                                                                                               | 1450                                                                                                                               | 1514                                                                                                                               | 350                                                                                     |
|         | CHAIN<br>ID          |                                                                               | B                                                                                                                                  | В                                                                                                                                  | В                                                                                                                                  | В                                                                                                                                  | В                                                                                       |
|         | PDB<br>ID            |                                                                               | 1qun                                                                                                                               | Iqun                                                                                                                               | 1qun                                                                                                                               | 1qun                                                                                                                               | 1qun                                                                                    |
|         | SEQ<br>D             | O                                                                             | 1706                                                                                                                               | 1706                                                                                                                               | 1706                                                                                                                               | 1706                                                                                                                               | 1706                                                                                    |

| Table 5   Score   Score   Score   Score   FIMH; CHAIN; B, D, F, H, J, L, N, C   P;                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |       |                      |                                                       |                                                                                                                                    | <del></del>                                                                                                                        |                                                                                                                                    |                                                                                                                                    |                                                                                                                              |
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| Table 5   Table 5   Table 5   Table 5   Table 5   Table 5   Table 6   Table 6   Table 6   Table 7   Table 6   Table 7   Table 7   Table 6   Table 7   Table 6   Table 7   Table 6   Table 7   Table 7   Table 7   Table 7   Table 8   Tabl |       | PDB annotation       | COMPLEMENTATION, 2<br>CHAPERONE/STRUCTURAL<br>PROTEIN | CHAPERONE/STRUCTURAL PROTEIN CHAPERONE ADHESIN DONOR STRAND COMPLEMENTATION, 2 CHAPERONE/STRUCTURAL PROTEIN                        | CHAPERONE/STRUCTURAL PROTEIN CHAPERONE ADHESIN DONOR STRAND COMPLEMENTATION, 2 CHAPERONE/STRUCTURAL PROTEIN                        | CHAPERONE/STRUCTURAL<br>PROTEIN CHAPERONE<br>ADHESIN DONOR STRAND<br>COMPLEMENTATION, 2<br>CHAPERONE/STRUCTURAL<br>PROTEIN         | CHAPERONE/STRUCTURAL PROTEIN CHAPERONE ADHESIN DONOR STRAND COMPLEMENTATION, 2 CHAPERONE/STRUCTURAL PROTEIN                        | CHAPERONE/STRUCTURAL<br>PROTEIN CHAPERONE<br>ADHESIN DONOR STRAND<br>COMPLEMENTATION, 2                                      |
| Tab   CHAIN   START   END   Psi   Verify   PMF                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |       | Compound             | FIMH; CHAIN: B, D, F, H, J, L, N, P;                  | PAPD-LIKE CHAPERONE FIMC;<br>CHAIN: A, C, E, G, I, K, M, O;<br>MANNOSE-SPECIFIC ADHESIN<br>FIMH; CHAIN: B, D, F, H, J, L, N,<br>P; | PAPD-LIKE CHAPERONE FIMC;<br>CHAIN: A, C, E, G, I, K, M, O;<br>MANNOSE-SPECIFIC ADHESIN<br>FIMH; CHAIN: B, D, F, H, J, L, N,<br>P; | PAPD-LIKE CHAPERONE FIMC;<br>CHAIN: A, C, E, G, I, K, M, O;<br>MANNOSE-SPECIFIC ADHESIN<br>FIMH; CHAIN: B, D, F, H, J, L, N,<br>P; | PAPD-LIKE CHAPERONE FIMC;<br>CHAIN: A, C, E, G, I, K, M, O;<br>MANNOSE-SPECIFIC ADHESIN<br>FIMH; CHAIN: B, D, F, H, J, L, N,<br>P; | PAPD-LIKE CHAPERONE FIMC;<br>CHAIN: A, C, E, G, I, K, M, O;<br>MANNOSE-SPECIFIC ADHESIN<br>FIMH; CHAIN: B, D, F, H, J, L, N, |
| PDB   CHAIN   START   END   Psi   Verify   PM                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | ole 5 | SEQ<br>FOLD<br>score |                                                       |                                                                                                                                    |                                                                                                                                    |                                                                                                                                    |                                                                                                                                    |                                                                                                                              |
| PDB   CHAIN   START   END   Psi                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | Tal   | PMF<br>score         |                                                       | -0.20                                                                                                                              | -0.19                                                                                                                              | -0.20                                                                                                                              | -0.19                                                                                                                              | -0.20                                                                                                                        |
| PDB   CHAIN   START   END                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |       | Verify<br>score      |                                                       | 0.16                                                                                                                               | 0.22                                                                                                                               | 0.09                                                                                                                               | 0.15                                                                                                                               | 0.01                                                                                                                         |
| 19DB   CHAIN   START   10   10   10   10   10   10   10   1                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |       | Psi<br>Blast         |                                                       | 6e-37                                                                                                                              | 1.1e-37                                                                                                                            | 9.6e-35                                                                                                                            | 2.4e-34                                                                                                                            | 7.2e-35                                                                                                                      |
| PDB CHAIN ID ID Iquin B Iquin B Iquin B Iquin B                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |       | END<br>AA            |                                                       | 693                                                                                                                                | 785                                                                                                                                | 837                                                                                                                                | 965                                                                                                                                | 1230                                                                                                                         |
| 10                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |       | START<br>AA          |                                                       | 414                                                                                                                                | 509                                                                                                                                | 558                                                                                                                                | 0.09                                                                                                                               | 925                                                                                                                          |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |       | CHAIN                |                                                       | В                                                                                                                                  | В                                                                                                                                  | В                                                                                                                                  | В                                                                                                                                  | В                                                                                                                            |
| SEQ ID NO: 1706 1706 1706 1706 1706 1706 1706                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |       | PDB<br>ID            |                                                       | Iqun                                                                                                                               | 1qun                                                                                                                               | 1qun                                                                                                                               | 1qun                                                                                                                               | 1qun                                                                                                                         |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |       | SEQ<br>U             |                                                       | 1706                                                                                                                               | 1706                                                                                                                               | 1706                                                                                                                               | 1706                                                                                                                               | 1706                                                                                                                         |

|         | PDB annotation |            | CHAPERONE/STRUCTURAL PROTEIN |                                          |              |              |                                       |                                          |                                       |                                       |                                       |                                          | CELL CYCLE REGULATION CELL CYCLE REGULATION HERPESVIRUS SAIMIRI, VIRAL CYCLIN | CELL DIVISION RCYCLIN H (RECOMBINANT); CYCLIN, CELL CYCLE, CELL DIVISION, NUCLEAR PROTEIN | COMPLEX (PROTEIN      |
|---------|----------------|------------|------------------------------|------------------------------------------|--------------|--------------|---------------------------------------|------------------------------------------|---------------------------------------|---------------------------------------|---------------------------------------|------------------------------------------|-------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------|-----------------------|
|         | Compound       |            | P;                           | VIRUS TOMATO BUSHY STUNT<br>VIRUS 2TBV 4 | VIRUS 2TBV 4 | VIRUS 2TBV 4 | VIRUS TOMATO BUSHY STUNT VIRUS 2TBV 4 | VIRUS TOMATO BUSHY STUNT<br>VIRUS 2TBV 4 | VIRUS TOMATO BUSHY STUNT VIRUS 2TBV 4 | VIRUS TOMATO BUSHY STUNT VIRUS 2TBV 4 | VIRUS TOMATO BUSHY STUNT VIRUS 2TBV 4 | VIRUS TOMATO BUSHY STUNT<br>VIRUS 2TBV 4 | CYCLIN HOMOLOG; CHAIN: A;                                                     | CYCLIN H; CHAIN: NULL;                                                                    | CELL DIVISION PROTEIN |
| Table 5 | SEQ            | FOLD       |                              |                                          |              |              |                                       |                                          |                                       |                                       |                                       |                                          | 54.78                                                                         | 65.17                                                                                     |                       |
| Tat     | PMF            | score      |                              | -0.20                                    | -0.19        | -0.19        | -0.19                                 | -0.18                                    | -0.18                                 | -0.20                                 | -0.20                                 | -0.20                                    |                                                                               |                                                                                           | 0.00                  |
|         | Verify         | score      |                              | 0.04                                     | 0.04         | 0.20         | 60.0                                  | 0.11                                     | 0.10                                  | 0.11                                  | 0.00                                  | 0.08                                     |                                                                               |                                                                                           | -0.50                 |
|         | Psi            | Blast      |                              | 9.6e-34                                  | 9.6e-40      | 1.2e-41      | 8.4e-37                               | 6e-23                                    | 1.2e-34                               | 1.2e-41                               | 6e-38                                 | 8.4e-33                                  | 4.4e-12                                                                       | 0.0022                                                                                    | 1.1e-10               |
|         | END            | ΑA         |                              | 1357                                     | 1568         | 1709         | 1888                                  | 433                                      | 529                                   | 705                                   | 1060                                  | 1326                                     | 273                                                                           | 304                                                                                       | 292                   |
|         | START          | AA         |                              | 1039                                     | 1253         | 1384         | 1577                                  | 173                                      | 249                                   | 377                                   | 733                                   | 985                                      | 49                                                                            | 31                                                                                        | 110                   |
|         | CHAIN          | О          |                              | O O                                      | C            | O            | C                                     | 0                                        | C                                     | S                                     | D D                                   | S                                        | Ą                                                                             |                                                                                           | В                     |
|         | PDB            | А          |                              | 2tbv                                     | 2tbv         | 2tbv         | 2tbv                                  | 2tbv                                     | 2tbv                                  | 2tbv                                  | 2tbv                                  | 2tbv                                     | 1bu2                                                                          | 1jkw                                                                                      | 1qmz                  |
|         | SEQ            | <br>百<br>复 |                              | 1706                                     | 1706         | 1706         | 1706                                  | 1706                                     | 1706                                  | 1706                                  | 1706                                  | 1706                                     | 1733                                                                          | 1733                                                                                      | 1733                  |

## WO 03/029271 PCT/US02/30474

|         |                      |                                                                           |                       |                                         |                                    |                         |                     |                 |                         |                     |                 | <br>                      |                      |                  |                     |                         | —т          |                          |                  |                  |                    |                 |         | -                                               |
|---------|----------------------|---------------------------------------------------------------------------|-----------------------|-----------------------------------------|------------------------------------|-------------------------|---------------------|-----------------|-------------------------|---------------------|-----------------|---------------------------|----------------------|------------------|---------------------|-------------------------|-------------|--------------------------|------------------|------------------|--------------------|-----------------|---------|-------------------------------------------------|
|         | PDB annotation       | KINASE/CYCLIN) CYCLIN-<br>DEPENDENT KINASE-2,<br>CDK2 P33 PROTEIN KINASE: | CCNA, CCN1; COMPLEX   | (PROTEIN KINASE/CYCLIN), CYCLIN, COK. 2 | PHOSPHORYLATION, SUBSTRATE COMPLEX | BINDING PROTEIN CYCLIN, | CELL CYCLE, KINASE- | BINDING PROTEIN | BINDING PROTEIN CYCLIN, | CELL CYCLE, KINASE- | BINDING PROTEIN | TRANSFERASE ATK,          | AMGX1, BPK; TYROSINE | KINASE, X-LINKED | AGAMMAGLOBULINEMIA, | XLA, BTK, SH3 2 DOMAIN, | TRANSFERASE | TRANSMEMBRANE            | PROTEIN COLICIN, | BACTERIOCIN, ION | CHANNEL FORMATION, | TRANSMEMBRANE 2 | PROTEIN |                                                 |
|         | Compound             | KINASE 2; CHAIN: A, C;<br>G2/MITOTIC-SPECIFIC CYCLIN                      | PEPTIDE; CHAIN: E, F; |                                         |                                    | CYCLIN A; CHAIN: NULL;  |                     |                 | CYCLIN A; CHAIN: NULL;  |                     |                 | BRUTON'S TYROSINE KINASE; | CHAIN: NULL;         |                  |                     |                         |             | COLICIN IA; CHAIN: NULL; |                  |                  |                    |                 |         | PHOSPHOTRANSFERASE C-SRC<br>KINASE (SH3 DOMAIN) |
| Table 5 | SEQ<br>FOLD<br>score |                                                                           |                       |                                         |                                    |                         |                     |                 | 56.74                   |                     |                 |                           |                      |                  |                     |                         |             | 76.29                    |                  |                  |                    |                 |         |                                                 |
| Tab     | PMF<br>score         |                                                                           |                       |                                         |                                    | 90.0                    |                     |                 |                         |                     |                 | 0.74                      |                      |                  |                     |                         | -           |                          |                  |                  |                    |                 |         | 0.99                                            |
|         | Verify<br>score      |                                                                           |                       |                                         |                                    | -0.65                   |                     |                 |                         |                     |                 | 0.87                      |                      |                  |                     |                         |             |                          |                  |                  |                    |                 |         | 69.0                                            |
|         | Psi<br>Blast         |                                                                           |                       |                                         |                                    | 8.8e-10                 |                     |                 | 8.8e-10                 | _                   |                 | 1.3e-12                   |                      |                  |                     |                         |             | 1.5e-05                  |                  |                  |                    |                 |         | 2.2e-13                                         |
|         | END                  |                                                                           |                       |                                         |                                    | 222                     |                     |                 | 313                     |                     |                 | 630                       | ·                    |                  |                     |                         |             | 614                      |                  |                  |                    |                 |         | 626                                             |
|         | START<br>AA          |                                                                           |                       |                                         |                                    | 110                     |                     |                 | 28                      | )                   | _               | 695                       |                      |                  |                     |                         |             | 35                       | 3                |                  |                    |                 |         | 574                                             |
|         | CHAIN<br>ID          |                                                                           |                       |                                         |                                    |                         |                     |                 |                         |                     |                 |                           |                      |                  |                     |                         |             |                          |                  |                  |                    |                 |         | A                                               |
|         | PDB<br>ID            |                                                                           |                       |                                         |                                    | 1vin                    | <br>!<br>:          |                 | 1vin                    |                     |                 | 1 aww                     | :                    |                  |                     |                         |             | 15:                      |                  |                  |                    | -               |         | 1csk                                            |
|         | SEQ<br>ID            |                                                                           | _                     |                                         |                                    | 1733                    | )                   | <del></del>     | 1733                    |                     |                 | 1734                      | 7                    |                  |                     |                         |             | 1734                     | 1                |                  |                    |                 |         | 1734                                            |

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| T. T | rds annotation       |                        | STRUCTURAL PROTEIN<br>TWO REPEATS OF | SPECTRIN, ALPHA HELICAL | LINKER REGION, 2.2<br>TANDEM 3-HELIX COILED- | COILS, STRUCTURAL | PROTEIN | TRANSFERASE PROTO-<br>ONCOGENE TYROSINE | KINASE; PROTO- | ONCOGENE, TRANSFERASE, | TYROSINE-PROTEIN | KINASE, 2<br>PHOSPHORYLATION. ATP- | BINDING, MYRISTYLATION, | SH3 DOMAIN, 3 COMPLEX | (PHOSPHOTRANSFERASE/PE | FILEDE) | COMPLEX (SIGNAL<br>TRANSDUCTION/PEPTIDE) | COMPLEX (SIGNAL | I KANSDUCTION/FEFTIME),<br>SH3 DOMAIN |                     |                                              |                          |                       |                                                       |  |
|------------------------------------------|----------------------|------------------------|--------------------------------------|-------------------------|----------------------------------------------|-------------------|---------|-----------------------------------------|----------------|------------------------|------------------|------------------------------------|-------------------------|-----------------------|------------------------|---------|------------------------------------------|-----------------|---------------------------------------|---------------------|----------------------------------------------|--------------------------|-----------------------|-------------------------------------------------------|--|
|                                          | Compound             | (E.C.2.7.1.112) 1CSK 3 | ALPHA SPECTRIN; CHAIN: A, B,         | ĵ.                      |                                              |                   |         | PHOSPHOTRANSFERASE FYN;                 |                |                        |                  |                                    |                         |                       |                        |         | GRB2; CHAIN: A; SOS-1; CHAIN:<br>B;      |                 |                                       | SIGNAL TRANSDUCTION | PROTEIN GROWTH FACTOR  PROTEIN GROWTH FACTOR | (GRB2, N-TERMINAL 1GBR 3 | SH3 DOMAIN) COMPLEXED | WITH SOS-A PEPTIDE 1GBR 4 (NMR, 29 STRUCTURES) 1GBR 5 |  |
| Table 5                                  | SEQ<br>FOLD<br>score |                        |                                      |                         |                                              |                   |         |                                         |                | -                      |                  |                                    |                         |                       |                        |         |                                          |                 |                                       |                     |                                              |                          |                       |                                                       |  |
| Tat                                      | PMF                  |                        | 0.10                                 |                         |                                              |                   |         | 0.95                                    |                |                        | _                |                                    |                         |                       |                        |         | 0.99                                     |                 |                                       | 0.88                |                                              |                          |                       |                                                       |  |
|                                          | Verify<br>score      |                        | 0.05                                 |                         |                                              |                   |         | 0.15                                    |                |                        |                  |                                    |                         |                       |                        |         | 0.73                                     |                 |                                       | 0.74                |                                              |                          |                       |                                                       |  |
|                                          | Psi<br>Blast         |                        | 2.2e-06                              |                         |                                              |                   |         | 4.4e-12                                 |                |                        |                  |                                    |                         |                       |                        |         | 6.6e-14                                  |                 |                                       | 1.3e-13             |                                              |                          |                       | . *.                                                  |  |
|                                          | END<br>AA            |                        | 242                                  |                         |                                              |                   |         | 626                                     |                |                        |                  |                                    |                         |                       |                        |         | 628                                      |                 |                                       | 628                 |                                              |                          |                       |                                                       |  |
|                                          | START                |                        | 63                                   |                         |                                              |                   |         | 574                                     |                |                        |                  |                                    |                         |                       |                        |         | 574                                      |                 |                                       | 266                 | )                                            |                          |                       |                                                       |  |
|                                          | CHAIN                |                        | A                                    |                         |                                              |                   |         | A                                       |                |                        |                  |                                    |                         |                       |                        |         | A                                        |                 |                                       | A                   | 1                                            |                          |                       |                                                       |  |
|                                          | PDB<br>ID            |                        | 1cun                                 |                         |                                              |                   |         | 1fyn                                    |                |                        |                  |                                    |                         |                       |                        |         | 1gbq                                     |                 |                                       | 1 ohr               | 1021                                         |                          |                       |                                                       |  |
|                                          | SEQ                  | SON C                  | 1734                                 |                         |                                              |                   |         | 1734                                    |                |                        |                  |                                    |                         |                       |                        |         | 1734                                     |                 |                                       | 1734                | t ( ) 1                                      |                          |                       |                                                       |  |

|         | PDB annotation  |                                                                                                                              | COMPLEX<br>(TRANSFERASE/PEPTIDE)<br>SRC, SH3 DOMAIN,<br>LIGANDS, NON-PEPTIDE<br>ELEMENTS, 2 COMPLEX<br>(TRANSFERASE/PEPTIDE)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | TYROSINE-PROTEIN KINASE BRUTONS TYROSINE KINASE, B CELL PROGENITOR KINASE, TRANSFERASE, TYROSINE- PROTEIN KINASE, PHOSPHORYLATION, 2 SH3 DOMAIN | TRANSFERASE HCK; SH3, PROTEIN TYROSINE KINASE, SIGNAL TRANSDUCTION, 2 TRANSFERASE | TRANSFERASE SHMT; HYDROXYMETHYL TRANSFERASE, 1 CARBON METABOLISM | LYASE CGS; LYASE, LLP-  |
|---------|-----------------|------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------|------------------------------------------------------------------|-------------------------|
|         | Compound        | PHOSPHORIC DIESTER HYDROLASE PHOSPHOLIPASE C-GAMMA (SH3 DOMAIN) (E.C.3.1.4.11) 1HSQ 3 (NMR, MINIMIZED MEAN STRUCTURE) 1HSQ 4 | C-SRC; CHAIN: C; NL1 (MN7- CO; MN2-MN1-PLPPLP); CHAIN: N; SR(R) SR(R) CHAIN: N; CHAIN: N; SR(R) CHAIN: N; CHAIN: | TYROSINE-PROTEIN KINASE TY BTK; CHAIN: A; TY TY PR TR DDC                                                         | HEMATOPOIETIC CELL KINASE; TR CHAIN: NULL; PR KII TR TR TR                        | ERA                                                              | CYSTATHIONINE GAMMA- LY |
| Table 5 | SEQ<br>FOLD     |                                                                                                                              |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |                                                                                                                                                 |                                                                                   |                                                                  |                         |
| I'a     | PMF             | 0.35                                                                                                                         | 66.0                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           | 0.87                                                                                                                                            | 96.0                                                                              | 0.17                                                             | 0.23                    |
|         | Verify<br>score | 0.58                                                                                                                         | 0.67                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           | 0.51                                                                                                                                            | 0.14                                                                              | -0.19                                                            | -0.28                   |
|         | Psi<br>Blast    | 2.2e-13                                                                                                                      | 8.8e-14                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        | 6.6e-12                                                                                                                                         | 6.6e-12                                                                           | 1.7e-30                                                          | 1.2e-14                 |
|         | END             | 636                                                                                                                          | 626                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            | 626                                                                                                                                             | 626                                                                               | 258                                                              | 185                     |
|         | START<br>AA     | 569                                                                                                                          | 573                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            | 571                                                                                                                                             | 574                                                                               | 26                                                               | 3                       |
|         | CHAIN           |                                                                                                                              | U                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | - A                                                                                                                                             |                                                                                   | A                                                                | A                       |
|         | PDB<br>ID       | 1hsq                                                                                                                         | Inlo                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           | 1qly                                                                                                                                            | 4hck                                                                              | 1cj0                                                             | 1cs1                    |
|         | SEQ<br>D        |                                                                                                                              | 1734                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           | 1734                                                                                                                                            | 1734                                                                              | 1750                                                             | 1750                    |

| _       |                      |                                                  |                                                                                             | - 1 |                                                              |                                                                                     |                                                                                     |                                                                                     | <del></del>                                                                         |                                                            |
|---------|----------------------|--------------------------------------------------|---------------------------------------------------------------------------------------------|-----|--------------------------------------------------------------|-------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|------------------------------------------------------------|
|         | PDB annotation       | DEPENDENT ENZYMES,<br>METHIONINE<br>BIOSYNTHESIS | TRANSFERASE SHMT, SERINE METHYLASE; ALPHA PLP ASPARTATE, AMINO TRANSFERASE, (AAT)-LIKE FOLD |     | IMMUNOGLOBULIN<br>IMMUNOGLOBULIN, C<br>REGION, V REGION      |                                                                                     |                                                                                     |                                                                                     |                                                                                     |                                                            |
|         | Compound             | SYNTHASE; CHAIN: A, B, C, D;                     | SERINE<br>HYDROXYMETHYLTRANSFERA<br>SE; CHAIN: A, B, C, D;                                  |     | ANTI-IDIOTYPIC FAB 409.5.3<br>(IGG2A) FAB; CHAIN: A, B, L, H | GLYCOSYLTRANSFERASE<br>CYCLODEXTRIN<br>GLYCOSYLTRANSFERASE<br>(E.C.2.4.1.19) 1CGT 3 | GLYCOSYLTRANSFERASE<br>CYCLODEXTRIN<br>GLYCOSYLTRANSFERASE<br>(E.C.2.4.1.19) 1CGT 3 | GLYCOSYLTRANSFERASE<br>CYCLODEXTRIN<br>GLYCOSYLTRANSFERASE<br>(E.C.2.4.1.19) 1CGT 3 | GLYCOSYLTRANSFERASE<br>CYCLODEXTRIN<br>GLYCOSYLTRANSFERASE<br>(E.C.2.4.1.19) 1CGT 3 | GLYCOSYLTRANSFERASE<br>CYCLODEXTRIN<br>GLYCOSYLTRANSFERASE |
| Table 5 | SEQ<br>FOLD<br>score |                                                  |                                                                                             |     |                                                              |                                                                                     |                                                                                     |                                                                                     |                                                                                     |                                                            |
| Tab     | PMF                  |                                                  | 0.10                                                                                        |     | 0.53                                                         | -0.11                                                                               | -0.15                                                                               | -0.15                                                                               | -0.15                                                                               | -0.15                                                      |
|         | Verify<br>score      |                                                  | 60.0                                                                                        |     | 0.33                                                         | 0.38                                                                                | 0.20                                                                                | 0.01                                                                                | 0.00                                                                                | 0.25                                                       |
|         | Psi<br>Blast         |                                                  | 3.4e-40                                                                                     |     | 0.0006                                                       | 4e-10 ~                                                                             | 4e-12                                                                               | 2e-12                                                                               | 2e-12                                                                               | 1e-12                                                      |
|         | END                  |                                                  | 255                                                                                         |     | 968                                                          | 1199                                                                                | 393                                                                                 | 476                                                                                 | 505                                                                                 | 561                                                        |
|         | START<br>AA          |                                                  | 2                                                                                           |     | 802                                                          | 1004                                                                                | 129                                                                                 | 221                                                                                 | 296                                                                                 | 352                                                        |
|         | CHAIN                |                                                  | A                                                                                           |     | Н                                                            |                                                                                     |                                                                                     |                                                                                     |                                                                                     |                                                            |
|         | PDB<br>ID            |                                                  | 1dfo                                                                                        |     | laif                                                         | legt                                                                                | legt                                                                                | lcgt                                                                                | lcgt                                                                                | 1cgt                                                       |
|         | SEQ<br>EQ            |                                                  | 1750                                                                                        |     | 1764                                                         | 1764                                                                                | 1764                                                                                | 1764                                                                                | 1764                                                                                | 1764                                                       |

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|         | PDB annotation |       |                       |                     |              |                     |                       |                     |               |                     |                       |                     |              |                     |                       |                     |              |                     |                       |                     |              |                     |                       |                     |              |                     |                       |                     |              |                     |                       |                                     |
|---------|----------------|-------|-----------------------|---------------------|--------------|---------------------|-----------------------|---------------------|---------------|---------------------|-----------------------|---------------------|--------------|---------------------|-----------------------|---------------------|--------------|---------------------|-----------------------|---------------------|--------------|---------------------|-----------------------|---------------------|--------------|---------------------|-----------------------|---------------------|--------------|---------------------|-----------------------|-------------------------------------|
|         | Compound       |       | (E.C.2.4.1.19) 1CGT 3 | GLYCOSYLTRANSFERASE | CYCLODEXTRIN | GLYCOSYLTRANSFERASE | (E.C.2.4.1.19) ICG1 3 | GLYCOSYLTRANSFERASE | CYCLODEAI KIN | GLYCOSYLIRANSFERASE | (E.C.2.4.1.19) ICGL 3 | GLYCOSYLTRANSFERASE | CYCLODEXTRIN | GLYCOSYLTRANSFERASE | (E.C.2.4.1.19) 1CGT 3 | GLYCOSYLTRANSFERASE | CYCLODEXTRIN | GLYCOSYLTRANSFERASE | (E.C.2.4.1.19) 1CGT 3 | GLYCOSYLTRANSFERASE | CYCLODEXTRIN | GLYCOSYLTRANSFERASE | (E.C.2.4.1.19) 1CGT 3 | GLYCOSYLTRANSFERASE | CYCLODEXTRIN | GLYCOSYLTRANSFERASE | (E.C.2.4.1.19) 1CGT 3 | GLYCOSYLTRANSFERASE | CYCLODEXTRIN | GLYCOSYLTRANSFERASE | (E.C.2.4.1.19) 1CGT 3 | GLYCOSYLTRANSFERASE<br>CYCLODEXTRIN |
| Table 5 | SEQ            | FOLD  |                       |                     |              |                     |                       |                     |               |                     |                       |                     |              |                     |                       |                     |              |                     |                       |                     |              |                     |                       |                     |              |                     |                       |                     |              |                     |                       |                                     |
| Tal     | PMF            | score |                       | -0.15               |              |                     |                       | -0.18               |               |                     |                       | -0.18               |              |                     |                       | -0.19               |              |                     |                       | -0.20               |              |                     |                       | -0.20               |              |                     |                       | -0.20               |              |                     |                       | -0.17                               |
|         | Verify         | score |                       | 0.32                |              |                     |                       | 0.10                |               |                     |                       | 0.10                |              |                     |                       | 0.18                |              |                     |                       | 90.0                |              |                     |                       | 0.19                |              |                     |                       | 0.30                |              | <u>-</u>            |                       | 0.24                                |
|         | Psi            | Blast |                       | 4e-16               |              |                     |                       | 1.6e-12             |               |                     |                       | 2e-10               |              |                     |                       | 6e-11               |              |                     |                       | 4e-12               |              |                     |                       | 6e-11               |              |                     |                       | 4e-14               |              |                     |                       | 1.4e-09                             |
|         | END            | AA    |                       | 617                 |              |                     |                       | 002                 |               |                     |                       | 283                 |              |                     |                       | 754                 |              |                     |                       | 841                 |              |                     |                       | 894                 |              |                     |                       | 943                 |              |                     |                       | 1007                                |
|         | START          | AA    |                       | 381                 |              |                     |                       | 430                 |               |                     |                       | 44                  |              |                     |                       | 512                 |              |                     |                       | 584                 |              |                     |                       | 684                 |              |                     |                       | 739                 | <u>.</u>     |                     |                       | 746                                 |
|         | CHAIN          |       |                       |                     |              |                     |                       |                     |               |                     |                       |                     |              |                     |                       |                     |              |                     |                       |                     |              |                     |                       |                     |              |                     |                       |                     |              |                     |                       |                                     |
|         | PDB            |       |                       | 1cgt                | 30           |                     |                       | 1cgt                |               |                     |                       | 1cgt                | )            |                     |                       | 1cot                |              |                     |                       | 1cot                | ,<br>,       |                     |                       | lcet                | <b>b</b>     |                     |                       | 1cot                | 3            |                     |                       | 1cgt                                |
|         | SEO            | í A Ş |                       | 1764                |              |                     |                       | 1764                |               |                     |                       | 1764                |              |                     |                       | 1764                |              |                     |                       | 1764                |              |                     |                       | 1764                |              |                     |                       | 1764                |              |                     |                       | 1764                                |

|         | PDB annotation       |                                              |                     |                                    | Account.              |                     |              |                                              |                     |              |                     |                       |                     |              |                     |                       | GLYCOSIDASE CGTASE; | 1CIU 8 THERMOSTABLE       | ICIO 14               | GLYCOSIDASE CGTASE; | ICIU 8 I HEKMUSIABLE<br>1CTI 14 | CI VOCITA OF CCTA OF. | GLICOSIDASE CUIASE;<br>1CIII & THFRMOSTABLE | ICHI 14              | GLYCOSIDASE CGTASE: | 1CIU 8 THERMOSTABLE       | 1CIU 14               | GLYCOSIDASE CGTASE; |
|---------|----------------------|----------------------------------------------|---------------------|------------------------------------|-----------------------|---------------------|--------------|----------------------------------------------|---------------------|--------------|---------------------|-----------------------|---------------------|--------------|---------------------|-----------------------|---------------------|---------------------------|-----------------------|---------------------|---------------------------------|-----------------------|---------------------------------------------|----------------------|---------------------|---------------------------|-----------------------|---------------------|
|         | Compound             | GLYCOSYLTRANSFERASE<br>(E.C.2.4.1.19) 1CGT 3 | GLYCOSYLTRANSFERASE | CYCLODEXTRIN GI VOOSVI TRANSFERASE | (E.C.2.4.1.19) 1CGT 3 | GLYCOSYLTRANSFERASE | CYCLODEXTRIN | GLYCOSYLTRANSFERASE<br>(E.C.2.4.1.19) 1CGT 3 | GLYCOSYLTRANSFERASE | CYCLODEXTRIN | GLYCOSYLTRANSFERASE | (E.C.2.4.1.19) 1CGT 3 | GLYCOSYLTRANSFERASE | CYCLODEXTRIN | GLYCOSYLTRANSFERASE | (E.C.2.4.1.19) 1CGT 3 | CYCLODEXTRIN        | GLYCOSYLTRANSFERASE; 1CIU | 6 CHAIN: NULL; ICIU / | CYCLODEXTRIN        | GLYCOSYLTRANSFERASE; ICIU       | OCHAIN: NOLL, IOIO /  | CYCLODEX I KIN                              | CELCOSTEINATOR, ICAC | CVCI ODEXTRIN       | GLYCOSYLTRANSFERASE: 1CTU | 6 CHAIN: NULL; 1CIU 7 | CYCLODEXTRIN        |
| Table 5 | SEQ<br>FOLD<br>score |                                              |                     |                                    |                       |                     |              |                                              |                     |              |                     |                       |                     |              |                     |                       |                     |                           |                       |                     |                                 |                       |                                             |                      |                     |                           |                       |                     |
| Tal     | PMF<br>score         |                                              | -0.12               |                                    |                       | -0.20               |              |                                              | -0.18               |              |                     |                       | -0.12               |              |                     |                       | -0.19               |                           |                       | -0.12               |                                 | ,                     | -0.19                                       |                      | -0 10               | ;                         |                       | -0.20               |
|         | Verify<br>score      |                                              | 0.45                |                                    |                       | 0.14                |              |                                              | 0.21                |              |                     |                       | 0.25                |              |                     |                       | 0.20                |                           |                       | 0.21                |                                 |                       | 0.22                                        |                      | 7,00                | 7.0                       |                       | 0.14                |
|         | Psi<br>Blast         |                                              | 6e-11               |                                    |                       | 1e-09               |              |                                              | 1.8e-11             |              |                     |                       | 1.2e-12             |              |                     |                       | 1.4e-24             |                           |                       | 1.4e-22             |                                 |                       | le-24                                       |                      | \$0.05              | 27-20                     |                       | 6e-26               |
|         | END<br>AA            |                                              | 203                 |                                    |                       | 1035                |              |                                              | 1090                | )<br>)       |                     |                       | 1155                |              |                     |                       | 434                 |                           |                       | 532                 |                                 |                       | 339                                         |                      | 264                 | t 000                     |                       | 643                 |
|         | START<br>AA          |                                              | 8                   |                                    |                       | 801                 |              |                                              | 830                 |              |                     |                       | 885                 |              |                     |                       | 124                 |                           |                       | 165                 |                                 |                       | 2                                           |                      | 101                 | 777                       |                       | 301                 |
|         | CHAIN                |                                              |                     |                                    |                       |                     |              |                                              |                     |              |                     |                       |                     |              |                     |                       |                     |                           |                       |                     |                                 |                       |                                             |                      |                     |                           |                       |                     |
|         | PDB<br>ID            |                                              | 1cgt                |                                    |                       | 1cot                | .0           |                                              | 1cot                | 1681         |                     |                       | legt                | )            | •                   |                       | 1ciu                |                           |                       | 1ciu                |                                 |                       | 1ciu                                        |                      |                     | ıcın                      |                       | 1ciu                |
|         | SEQ<br>EQ            | 5                                            | 1764                |                                    |                       | 1764                |              |                                              | 1764                |              |                     |                       | 1764                |              |                     | _                     | 1764                |                           |                       | 1764                |                                 |                       | 1764                                        |                      | 1707                | 1/04                      |                       | 1764                |

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|         | PDB annotation |          | ICIU 8 THERMOSTABLE<br>ICIU 14                  | GLYCOSIDASE CGTASE; | ICIU 8 THERMOSTABLE<br>ICIU 14                     | GLYCOSIDASE CGTASE; | 1CIU 8 THERMOSTABLE       | OT STOCKED A OF COTTA OF | GLYCOSIDASE CGIASE;<br>ICIII & THERMOSTABLE | 1CIU 14               | GLYCOSIDASE CGTASE; | 1CIU 8 THERMOSTABLE       | 1CIU 14               | GLYCOSIDASE CGTASE; | <b>ICIU 8 THERMOSTABLE</b> | 1CIU 14               | GLYCOSIDASE CGTASE; | 1CIU 8 THERMOSTABLE       | GI VCOSIDASE CGTASE: | 1CH S THERMOSTABLE | 1CIU 14               | GLYCOSIDASE CGTASE; | 1CIU 8 THERMOSTABLE       | 1CIU 14               | STRUCTURAL PROTEIN | INTEGRIN-BINDING<br>PROTEIN, INV GENE | STRUCTURAL PROTEIN | IN I EUKIN-DINDING |
|---------|----------------|----------|-------------------------------------------------|---------------------|----------------------------------------------------|---------------------|---------------------------|--------------------------|---------------------------------------------|-----------------------|---------------------|---------------------------|-----------------------|---------------------|----------------------------|-----------------------|---------------------|---------------------------|----------------------|--------------------|-----------------------|---------------------|---------------------------|-----------------------|--------------------|---------------------------------------|--------------------|--------------------|
|         | Compound       |          | GLYCOSYLTRANSFERASE; 1CIU 6 CHAIN: NULL: 1CIU 7 | CYCLODEXTRIN        | GLYCOSYLTRANSFERASE; 1CIU<br>6 CHAIN: NULL; 1CIU 7 | CYCLODEXTRIN        | GLYCOSYLTRANSFERASE; 1CIU | 6 CHAIN: NULL; ICIU /    | CYCLODEXTRIN GI VCOSVI TR ANSFER ASF: 10111 | 6 CHAIN: NULL: 1CIU 7 | CYCLODEXTRIN        | GLYCOSYLTRANSFERASE; 1CIU | 6 CHAIN: NULL; 1CIU 7 | CYCLODEXTRIN        | GLYCOSYLTRANSFERASE; 1CIU  | 6 CHAIN: NULL; 1CIU 7 | CYCLODEXTRIN        | GLYCOSYLTRANSFERASE; 1CIU | OVER OPENTRIN        | CICLODEAIMIN       | 6 CHAIN: NULL; 1CIU 7 | CYCLODEXTRIN        | GLYCOSYLTRANSFERASE; 1CIU | 6 CHAIN: NULL; 1CIU 7 | INVASIN; CHAIN: A; |                                       | INVASIN; CHAIN: A; |                    |
| Table 5 | SEQ            | FOLD     | -                                               |                     |                                                    |                     |                           |                          |                                             |                       |                     |                           |                       |                     |                            |                       |                     |                           |                      |                    |                       |                     |                           |                       |                    |                                       |                    |                    |
| Tat     | FMF            | score    |                                                 | -0 19               |                                                    | -0 14               |                           |                          | -0.19                                       |                       | -0.12               | ;                         |                       | -0.20               |                            |                       | -0.20               |                           | 6                    | 07:0-              |                       | -0.19               |                           |                       | -0.19              |                                       | -0.19              |                    |
|         | Verify         | score    |                                                 | 0.21                |                                                    | 0.16                | 3                         |                          | 0.24                                        |                       | 0.39                | )<br>}                    |                       | 0.22                |                            |                       | 0.23                |                           |                      | 0.12               |                       | 0.15                | ;                         |                       | 0.33               |                                       | 0.25               |                    |
|         | Psi            | Blast    |                                                 | 1 8e-24             |                                                    | 40.76               | 27-21                     |                          | 4e-24                                       |                       | 76-27               | 1                         |                       | 8e-23               |                            |                       | 6e-25               | <b> </b>                  |                      | 7e-72              |                       | 46-10               | 2                         |                       | 4e-53              |                                       | 1.4e-51            |                    |
|         | END            | AA       |                                                 | 700                 | 3                                                  | 8/11                |                           |                          | 863                                         |                       | 1007                |                           |                       | 475                 | )<br>-                     |                       | 1040                | )                         | ,                    | 1126               |                       | 1107                | ,,,,,                     |                       | 532                |                                       | 669                |                    |
|         | START          | AA       |                                                 | 308                 | 27                                                 | 121                 | 100                       |                          | 503                                         |                       | 503                 | 770                       |                       | 73                  | )                          |                       | 732                 | 1                         |                      | 268                |                       | 047                 | È                         |                       | 18                 |                                       | 193                |                    |
|         | CHAIN          | А        |                                                 |                     |                                                    |                     |                           |                          |                                             |                       |                     |                           |                       |                     |                            |                       |                     |                           |                      |                    |                       |                     |                           |                       | A                  | 1                                     | A                  |                    |
|         | PDB            | <u>a</u> |                                                 | 10::1               | n con                                              | 1.0                 | ıcın                      | -                        | 1ciu                                        |                       | 19:1                | n cin                     |                       | 1cin                | nior                       |                       | 1cin                | nicia                     |                      | 1ciu               |                       | 10in                | ncor                      |                       | 1cwv               |                                       | Icwv               |                    |
|         | SEQ            | ΒŞ       | j.                                              | ╁                   | 1/04                                               | 1764                | 1/04                      |                          | 1764                                        |                       | 1761                | +0/1<br>+0/1              |                       | 1761                | 1/04                       |                       | 1764                | t 0/1                     |                      | 1764               |                       | 1764                | 1/04                      |                       | 1764               |                                       | 1764               |                    |

|         | PDB annotation |       | PROTEIN, INV GENE | STRUCTURAL PROTEIN | PROTEIN, INV GENE | STRUCTURAL PROTEIN | INTEGRIN-BINDING | PROTEIN, INV GENE | STRUCTURAL PROTEIN | INTEGRIN-BINDING | PROTEIN, INV GENE | STRUCTURAL PROTEIN | INTEGRIN-BINDING | PROTEIN, INV GENE | STRUCTURAL PROTEIN | INTEGRIN-BINDING | PROTEIN, INV GENE | STRUCTURAL PROTEIN | NTEGRIN-BINDING | PROTEIN, INV GENE | STRUCTURAL PROTEIN | INTEGRIN-BINDING | FROI EIN, INV GENE | STRUCTURAL PROTEIN | PROTEIN, INV GENE |                     |              |                    |                                |                                     |   |
|---------|----------------|-------|-------------------|--------------------|-------------------|--------------------|------------------|-------------------|--------------------|------------------|-------------------|--------------------|------------------|-------------------|--------------------|------------------|-------------------|--------------------|-----------------|-------------------|--------------------|------------------|--------------------|--------------------|-------------------|---------------------|--------------|--------------------|--------------------------------|-------------------------------------|---|
|         | Compound       |       |                   | INVASIN; CHAIN: A; |                   | INVASIN; CHAIN: A; |                  | !                 | INVASIN; CHAIN: A; |                  |                   | INVASIN; CHAIN: A; |                  |                   | INVASIN; CHAIN: A; |                  |                   | INVASIN; CHAIN: A; |                 |                   | INVASIN; CHAIN: A; |                  |                    | INVASIN; CHAIN: A; |                   | GLYCOSYLTRANSFERASE | CYCLODEXTRIN | GLUCANOTRANSFERASE | (E.C.2.4.1.19) (CGTASE) 1CYG 3 | GLYCOSYLTRANSFERASE<br>CYCLODEXTRIN |   |
| Table 5 | SEQ            | score |                   |                    |                   |                    |                  |                   | 105.80             |                  |                   |                    |                  |                   |                    |                  |                   |                    |                 |                   |                    |                  |                    |                    |                   |                     |              |                    |                                |                                     |   |
| Ta      | PMF            | 2002  |                   | -0.18              |                   | -0.19              |                  |                   |                    |                  |                   | -0.20              |                  |                   | -0.18              |                  |                   | -0.17              |                 |                   | -0.19              |                  |                    | -0.20              |                   | -0.19               |              |                    |                                | -0.20                               | - |
|         | Verify         | 3000  |                   | 0.23               |                   | 0.40               |                  |                   |                    |                  |                   | 0.27               |                  |                   | 0.28               |                  |                   | 0.39               |                 |                   | 0.28               |                  |                    | 0.24               |                   | 0.21                | į<br>į       |                    |                                | 0.13                                |   |
|         | Psi<br>Rlast   | Diast |                   | 4e-52              |                   | 4e-54              |                  |                   | 4e-54              |                  | •                 | 8e-54              |                  |                   | le-52              |                  |                   | 1e-50              |                 |                   | 4e-35              |                  |                    | 4e-52              |                   | 1 2e-27             | 1            |                    |                                | 2e-16                               |   |
|         | END            |       |                   | 783                |                   | 883                |                  |                   | 948                |                  |                   | 1006               |                  |                   | 1001               |                  |                   | 1175               |                 |                   | 1196               |                  |                    | 638                |                   | 587                 | ,            |                    |                                | 204                                 |   |
|         | START          | WW.   |                   | 281                |                   | 364                |                  |                   | 445                |                  |                   | 493                | <u>.</u>         |                   | 613                | )                |                   | 029                | )               |                   | 998                |                  |                    | 86                 |                   | 125                 | 771          |                    |                                | 2                                   |   |
|         | CHAIN          | <br>] |                   | A                  |                   | A                  | 4                |                   | A                  |                  |                   | A                  | •                | _                 | 4                  | 4                |                   | d                  | 4               |                   | A                  |                  |                    | A                  |                   |                     |              |                    |                                |                                     |   |
|         | PDB            |       |                   | 1cwv               | _                 | 1cwv               |                  |                   | 1cwv               |                  |                   | 1cwv               |                  | •                 | 1cwv               |                  |                   | 1cwv               | :               |                   | 1cwv               |                  |                    | lcwv               |                   | 10370               | 1578         |                    |                                | 1cyg                                |   |
|         | SEQ            | E Ç   |                   | 1764               |                   | 1764               |                  |                   | 1764               |                  |                   | 1764               | 5                |                   | 1764               | 5                |                   | 1764               | 5               |                   | 1764               |                  |                    | 1764               |                   | 1764                | † 0 / I      |                    |                                | 1764                                |   |

|         | PDB annotation |       |                                                     |                                     |                                                      |                     |                                                      |                     |              |                                                      |                     |              |                    |                                |                     |                |                                | TRANSFERASE ALPHA- | AMYLASE, PRODUCT     | ONIFIEA,  | OLIGOSACCHARDE,<br>  FAMILY 13.2 GLYCOSYL | HYDROLASE, | TRANSGLYCOSYLATION, | INDUCED FIL, 3 CALALYS<br>TRANSFERASE |  |
|---------|----------------|-------|-----------------------------------------------------|-------------------------------------|------------------------------------------------------|---------------------|------------------------------------------------------|---------------------|--------------|------------------------------------------------------|---------------------|--------------|--------------------|--------------------------------|---------------------|----------------|--------------------------------|--------------------|----------------------|-----------|-------------------------------------------|------------|---------------------|---------------------------------------|--|
|         | Compound       |       | GLUCANOTRANSFERASE<br>(E.C.2.4.1.19) (CGTASE) 1CYG3 | GLYCOSYLTRANSFERASE<br>CYCLODEXTRIN | GLUCANOTRANSFERASE<br>(E.C.2.4.1.19) (CGTASE) 1CYG 3 | GLYCOSYLTRANSFERASE | GLUCANOTRANSFERASE<br>(E.C.2.4.1.19) (CGTASE) 1CYG 3 | GLYCOSYLTRANSFERASE | CYCLODEXTRIN | GLUCANOTRANSFERASE<br>(E.C.2.4.1.19) (CGTASE) 1CYG 3 | GLYCOSYLTRANSFERASE | CYCLODEXTRIN | GLUCANOTRANSFERASE | (E.C.2.4.1.19) (CGTASE) 1CYG 3 | GLYCOSYLTRANSFERASE | CYCLODEX I KIN | (E.C.2.4.1.19) (CGTASE) 1CYG 3 | CYCLODEXTRIN       | GLYCOSYLTRANSFERASE; | CHAIN: A; |                                           |            |                     |                                       |  |
| Table 5 | SEQ            | FOLD  |                                                     |                                     |                                                      |                     |                                                      |                     |              |                                                      |                     |              |                    |                                |                     |                |                                |                    |                      |           |                                           |            |                     |                                       |  |
| Ta      | PMF            | score |                                                     | -0.20                               |                                                      | -0.19               |                                                      | -0.19               |              |                                                      | -0.20               |              |                    |                                | -0.18               |                |                                | 0.05               |                      |           |                                           |            |                     |                                       |  |
|         | Verify         | score |                                                     | 0.01                                |                                                      | 0.33                |                                                      | 0.33                |              |                                                      | 0.15                |              |                    |                                | 0.21                |                |                                | 0.23               |                      |           |                                           |            |                     |                                       |  |
|         | Psi            | Blast |                                                     | 6e-28                               |                                                      | 4e-30               |                                                      | 1.2e-29             |              |                                                      | 1e-37               |              |                    |                                | 2e-20               |                |                                | 6e-10              |                      |           |                                           |            |                     |                                       |  |
|         | END            | AA    |                                                     | 476                                 |                                                      | 691                 |                                                      | 898                 | )            |                                                      | 1015                |              |                    |                                | 1197                |                |                                | 476                |                      |           |                                           |            |                     |                                       |  |
|         | START          | AA    |                                                     | 23                                  |                                                      | 243                 |                                                      | 456                 | 2            |                                                      | 548                 |              |                    |                                | 761                 |                |                                | 218                |                      |           |                                           |            |                     |                                       |  |
|         | CHAIN          | Э     |                                                     |                                     |                                                      |                     |                                                      |                     |              |                                                      |                     |              |                    |                                |                     |                |                                | A                  |                      |           |                                           |            |                     |                                       |  |
|         | PDB            | 日     |                                                     | 1cyg                                |                                                      | 1cyg                |                                                      | 1000                | 10,78        |                                                      | 1cvg                |              |                    |                                | 1cyg                | :              |                                | 1d3c               |                      |           |                                           |            |                     |                                       |  |
|         | SEQ            | ́ДŞ   | 5                                                   | 1764                                |                                                      | 1764                |                                                      | 1764                | †<br>5       |                                                      | 1764                |              |                    |                                | 1764                |                |                                | 1764               |                      |           |                                           |            |                     |                                       |  |

| 1 6     | PIJB annotation | TRANSFERASE ALPHA- | AMYLASE, PRODUCT<br>COMPLEX,      | OLIGOSACCHARIDE, | FAMILY 13 2 GLYCOSYL | HYDROLASE, | TRANSGLYCOSYLATION, | TRANSFERASE | TRANSFERASE ALPHA- | AMYLASE, PRODUCT     | COMPLEA,  | OLIGOSACCHARIDE, | FAMILY 13.2 GLYCOSYL | HYDROLASE, | TRANSGLYCOSYLATION, | INDUCED FIT, 3 CATALYSIS, | TRANSFERASE | TRANSFERASE ALPHA- | AMYLASE, PRODUCT     | COMPLEX,  | OLIGOSACCHARIDE, | FAMILY 13 2 GLYCOSYL | HYDROLASE, | TRANSGLYCOSYLATION, | INDUCED FIT, 3 CATALYSIS, | TRANSFERASE | TRANSFERASE ALPHA- | AMYLASE, PRODUCT     | COMPLEX,      | ULIUUSINCCIIIIIIII) |
|---------|-----------------|--------------------|-----------------------------------|------------------|----------------------|------------|---------------------|-------------|--------------------|----------------------|-----------|------------------|----------------------|------------|---------------------|---------------------------|-------------|--------------------|----------------------|-----------|------------------|----------------------|------------|---------------------|---------------------------|-------------|--------------------|----------------------|---------------|---------------------|
|         | Compound        | CYCLODEXTRIN       | GLYCOSYLTRANSFERASE;<br>CHAIN: A: |                  |                      |            |                     |             | CYCLODEXTRIN       | GLYCOSYLTRANSFERASE; | CHAIN: A; |                  |                      |            |                     |                           |             | CYCLODEXTRIN       | GLYCOSYLTRANSFERASE; | CHAIN: A; |                  |                      |            |                     |                           |             | CYCLODEXTRIN       | GLYCOSYLTRANSFERASE; | CHAIN: A;     |                     |
| e 5     | SEQ<br>FOLD     | score              |                                   | -                |                      |            |                     |             |                    |                      |           |                  |                      |            |                     |                           |             |                    |                      |           |                  |                      |            |                     |                           |             |                    |                      |               |                     |
| Table 5 | FMF<br>score    | -0 14              |                                   |                  |                      |            |                     |             | -0.19              |                      |           |                  | -                    |            |                     |                           |             | -0.20              | )<br>!               |           |                  |                      |            | _                   |                           |             | -0.18              |                      |               |                     |
|         | Verify score    | 0.52               | 1                                 |                  |                      |            |                     |             | 0.20               |                      |           |                  |                      |            |                     |                           |             | 0.22               | 1                    |           |                  |                      |            |                     |                           |             | 0.21               |                      |               |                     |
|         | Psi<br>Blast    | 26.10              |                                   |                  |                      |            |                     |             | 4e-08              |                      |           |                  |                      |            |                     |                           |             | 46-00              |                      |           |                  |                      |            |                     |                           |             | 1.2e-08            |                      |               |                     |
|         | END             | 617                |                                   | _                |                      |            |                     |             | 841                |                      |           |                  |                      |            |                     |                           |             | 1080               |                      |           |                  |                      |            |                     |                           |             | 1124               |                      |               |                     |
|         | START<br>AA     | 270                |                                   |                  |                      |            |                     |             | 295                |                      |           |                  |                      |            |                     |                           | _           | 817                | /10                  |           |                  |                      |            |                     |                           |             | 698                | 3                    |               |                     |
|         | CHAIN           |                    | ₹                                 |                  |                      |            |                     | ,           |                    | ***                  |           |                  |                      |            |                     |                           |             |                    |                      |           |                  |                      |            |                     |                           |             | A                  | 4                    | _             |                     |
|         | PDB (           |                    | ldsc —                            |                  |                      |            |                     |             | 1,430              |                      |           |                  |                      |            |                     |                           |             | 1,420              |                      |           |                  |                      |            | _                   | _                         |             | 1430               | 3                    | <del></del> , |                     |
|         | SEQ             |                    |                                   |                  |                      | ,          |                     |             | 1764               |                      |           |                  |                      |            |                     |                           |             |                    | 1/04                 |           |                  |                      |            |                     |                           |             | 1764               | 5                    |               |                     |

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|         | PDB annotation |         | FAMILY 13 2 GLYCOSYL | TRANSGLYCOSYLATION, | INDUCED FIT, 3 CATALYSIS, | TRANSFERASE | TRANSFERASE ALPHA- | AMYLASE, PRODUCT     | COMPLEX,  | EANTEN 12 2 CT VCOGVI | FAIMIL I 13 Z GLI COS I L | HYDROLASE, | IRANSGLYCOSYLATION, | INDUCED FIT, 3 CATALYSIS, | TRANSFERASE | HYDROLASE               | NEURAMINIDASE; | HYDROLASE, | GLYCOSIDASE | HYDROLASE               |       | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
|         | Compound       |         |                      |                     |                           |             | CYCLODEXTRIN       | GLYCOSYLTRANSFERASE; | CHAIN: A; |                       |                           |            |                     |                           |             | SIALIDASE; CHAIN: NULL; |                |            |             | SIALIDASE; CHAIN: NULL; |                |            |             | SIALIDASE; CHAIN: NULL; |                |            |             | SIALIDASE; CHAIN: NULL; |                |            |             | SIALIDASE; CHAIN: NULL; |       |
| Table 5 | SEQ<br>FOI D   | score   |                      |                     |                           |             |                    |                      |           |                       |                           |            |                     |                           |             |                         |                |            |             |                         |                |            |             |                         |                |            | •           |                         |                |            |             |                         |       |
| Tat     | FMF            | 20026   |                      |                     |                           |             | -0.19              |                      |           |                       |                           |            |                     |                           |             | -0.19                   |                |            |             | -0.20                   |                |            |             | -0.20                   |                |            |             | -0.18                   |                |            |             | -0.19                   | ;     |
|         | Verify         | SCOTE   |                      |                     |                           |             | 0.08               | )<br>)<br>;          |           |                       |                           |            |                     |                           |             | 0.05                    | :              |            |             | 0.32                    | !              |            |             | 0.33                    |                |            |             | 0.36                    | )<br>!         |            |             | 0.31                    |       |
|         | Psi<br>Dlast   | Diasi   |                      |                     |                           |             | 4e-09              | )<br>)               |           |                       |                           |            |                     |                           |             | 1 fe-16                 |                |            |             | 1.6e-18                 |                |            |             | 2e-16                   |                |            |             | 1 2e-16                 |                |            |             | 1.6e-18                 | 71 77 |
|         | END            | HA<br>H |                      |                     |                           |             | 340                | 2                    |           |                       |                           |            |                     |                           |             | 737                     | 1              |            |             | 464                     | -              |            |             | 617                     |                |            |             | 411                     | 1              |            |             | 765                     | 3     |
|         | START          | AA<br>— |                      |                     |                           |             | 88                 | 3                    |           |                       |                           |            |                     |                           |             | 17                      | `              |            |             | 190                     | 2              |            |             | 190                     |                |            |             | 33                      | ì              |            |             | 365                     | 200   |
|         | CHAIN          |         |                      |                     |                           |             | V                  | ď                    |           |                       |                           |            |                     |                           |             |                         |                |            |             |                         |                |            |             |                         |                |            |             |                         |                |            |             |                         |       |
|         | PDB            | —<br>Э  |                      |                     |                           |             | 1430               | 701                  |           |                       |                           | ,          |                     |                           |             | 1 put                   | Tout           |            |             | 1 Punt                  | not -          |            |             | 1eut                    |                |            |             | 1 and                   | ınoı           |            |             | 10114                   | ıcnı  |
|         | SEQ            | <br>∋   | į                    |                     |                           |             | 1761               | t 0/1                |           |                       |                           |            |                     |                           |             | 1761                    | †<br>0/1       |            |             | 1761                    | + O / T        |            |             | 1764                    |                |            |             | 1764                    | t .            |            |             | 1764                    | 1/04  |

Table 5

|         | Compound           |             |
|---------|--------------------|-------------|
| Fable 5 | Psi Verify PMF SEQ | FOLD        |
| Tal     | FMF                | Score       |
|         | Verify             | Score Score |
|         | Psi                | Rlact       |
|         | END                | V V         |
|         | START              | <           |
|         | AIN                |             |

|         |                 |                      |                              |             |                         |                |            |             |                         |                |            |             |                         |                |            |             |                         |                |            |             |                         |                |            |             |                         |                |            |             |                     |                     |                                           | 1 |
|---------|-----------------|----------------------|------------------------------|-------------|-------------------------|----------------|------------|-------------|-------------------------|----------------|------------|-------------|-------------------------|----------------|------------|-------------|-------------------------|----------------|------------|-------------|-------------------------|----------------|------------|-------------|-------------------------|----------------|------------|-------------|---------------------|---------------------|-------------------------------------------|---|
|         | PDB annotation  | METER ANGENITY A CE. | NEUKAMINIDASE;<br>HYDROLASE, | GLYCOSIDASE | HYDROLASE               | NEURAMINIDASE; | HYDROLASE, | GLYCOSIDASE | GLYCOSYLTRANSFERASE | TRANSFERASE,        | GLYCOSYLTRANSFERASE,<br>  CALCIUM, SIGNAL | , |
|         | Compound        |                      |                              |             | SIALIDASE; CHAIN: NULL; |                |            |             | SIALIDASE; CHAIN: NULL; |                |            |             | SIALIDASE; CHAIN: NULL; |                |            |             | SIALIDASE; CHAIN: NULL; |                |            |             | SIALIDASE; CHAIN: NULL; |                |            |             | SIALIDASE; CHAIN: NULL; |                |            |             | CYCLODEXTRIN        | GLUCANOTRANSFERASE; | CHAIN: A, B;                              |   |
| Table 5 | SEQ<br>FOLD     | score                |                              |             |                         |                |            |             |                         |                |            |             | 151.40                  |                |            |             |                         |                |            |             |                         |                |            |             |                         |                |            |             |                     |                     |                                           |   |
| Tab     | PMF<br>score    |                      |                              |             | -0.15                   |                |            |             | -0.20                   |                |            |             |                         |                |            |             | -0.20                   |                |            |             | -0.17                   |                |            |             | -0.19                   |                |            |             | -0.20               |                     |                                           |   |
|         | Verify<br>score |                      |                              |             | 0.39                    |                |            |             | 0.33                    |                |            |             |                         |                |            |             | 0.21                    | 1              |            |             | 0.22                    |                |            |             | 0.36                    |                |            |             | 0.40                |                     |                                           |   |
|         | Psi<br>Blast    |                      | ***                          |             | 2e-20                   | ì              |            |             | 4e-20                   |                |            |             | 1 2e-18                 | 2              |            |             | 2e-18                   | 2              |            |             | 1.2e-18                 |                |            |             | 4e-17                   |                |            |             | 6e-33               |                     |                                           |   |
|         | END             |                      |                              |             | 854                     |                |            |             | 371                     |                |            |             | 1198                    | 2              |            |             | 666                     | 777            |            |             | 1145                    | )<br>•         |            |             | 1185                    | )<br>1         |            |             | 574                 |                     |                                           |   |
|         | START           |                      |                              |             | 501                     | 100            |            |             | 09                      |                |            |             | 900                     |                |            |             | 959                     | 2              |            |             | 693                     | )              |            |             | 766                     | 2              |            |             | 153                 | )<br>}              |                                           |   |
|         | CHAIN           |                      |                              |             |                         |                |            |             |                         |                |            |             |                         |                |            |             |                         |                |            |             |                         |                |            |             |                         |                |            |             | ٨                   | 4                   |                                           |   |
|         | PDB<br>ID       |                      |                              |             | 1 pint                  | Tent           |            |             | 1eut                    |                |            |             | 1 cm+                   | Tem            |            |             | 1 ant                   | ınaı           |            |             | 1011t                   | i ca           |            |             | four                    | inor           |            |             | lnam                | The last            |                                           |   |
|         | SEQ<br>ID       | NO:                  |                              |             | 1764                    | 1,04           |            |             | 1764                    |                |            |             | 1764                    | 1/04           |            |             | 1764                    | 1/04           |            |             | 1761                    | 1,01           |            |             | 1764                    | 101            |            |             | 1764                | 5                   |                                           |   |

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|---------|----------------|------------|-------------------------------------|----------------------|-----------------|------------------------------------|----------------------|-----------------|---------------------|---------------------|----------------------|-----------------------|-------------------------------------|----------------------|-----------------|---------------------|---------------------|----------------------|-----------------|---------------------|---------------------|----------------------|----------------------------|-----------------------|------------------|----------------------------|-------------------------------|--------------------------|-----------------------------------|
|         | PDB annotation |            | GLYCOSYLTRANSFERASE<br>TRANSFERASE, | GLYCOSYLTRANSFERASE, | CALCIUM, SIGNAL | GLYCOSYLTRANSFERASE<br>TRANSFERASE | GLYCOSYLTRANSFERASE, | CALCIUM, SIGNAL | GLYCOSYLTRANSFERASE | TRANSFERASE,        | GLYCOSYLTRANSFERASE, | GI VCOSVI TRANSFERASE | TRANSFERASE.                        | GLYCOSYLTRANSFERASE, | CALCIUM, SIGNAL | GLYCOSYLTRANSFERASE | TRANSFERASE,        | GLYCOSYLTRANSFERASE, | CALCIUM, SIGNAL | GLYCOSYLTRANSFERASE | TRANSFERASE,        | GLYCOSYLTRANSFERASE, | HVDROI ASE DOUBLE BETA     | A A D D TO THE DIAL   | SAKKEL, BACIEMAL | CHAPFRONE/STRUCTURAL       | PROTEIN CHAPERONE             | ADHESIN DONOR STRAND     | COMPLEMENTATION, 2                |
|         | Compound       |            | CYCLODEXTRIN<br>GLUCANOTRANSFERASE; | CHAIN: A, B;         |                 | CYCLODEXTRIN                       | CHAIN: A, B;         |                 | CYCLODEXTRIN        | GLUCANOTRANSFERASE; | CHAIN: A, B;         | CVCIODEVTBIN          | CICLODEAININ<br>GITTCANOTRANSFERASE | CHAIN: A. B.         |                 | CYCLODEXTRIN        | GLUCANOTRANSFERASE; | CHAIN: A, B;         | :               | CYCLODEXTRIN        | GLUCANOTRANSFERASE; | CHAIN: A, B;         | AT DITA T WHICH DECIDENCE. | ALPHA-LIIIC FNOIEASE, | CHAIN: A;        | BABD I IKE CHAPERONE FIMC: | CHAIN: A C. F. G. I. K. M. O. | MANNOSE-SPECIFIC ADHESIN | FIMH; CHAIN: B, D, F, H, J, L, N, |
| le 5    | SEQ            | FOLD score |                                     |                      |                 |                                    |                      |                 |                     |                     |                      |                       |                                     |                      |                 |                     |                     |                      |                 |                     |                     |                      |                            |                       |                  |                            |                               |                          |                                   |
| Table 5 | PMF            | score      | -0.19                               |                      |                 | -0.20                              |                      |                 | -0.19               |                     |                      | 6                     | -0.20                               |                      |                 | -0.20               |                     |                      |                 | -0.17               |                     |                      | 3                          | 0.04                  |                  | 000                        | 70.40                         |                          |                                   |
|         | Verify         | score      | 0.22                                |                      |                 | 0.23                               |                      |                 | 0.39                |                     |                      |                       | 07.0                                |                      |                 | 0.17                |                     |                      |                 | 0.30                |                     |                      | 0                          | 0.70                  |                  | 30.0                       | رع.٥                          |                          |                                   |
|         | Psi            | Blast      | 8e-30                               |                      |                 | 6e-33                              |                      |                 | 8e-33               |                     |                      |                       | 6e-33                               |                      |                 | 8e-32               |                     |                      |                 | 8e-30               |                     |                      |                            | 1.6e-05               |                  | 1 0 10                     | 01-20-1                       |                          |                                   |
|         | END            | AA         | 620                                 |                      |                 | 841                                | -                    |                 | 884                 |                     |                      |                       | 1007                                |                      |                 | 1159                |                     |                      |                 | 382                 | -                   |                      |                            | 962                   |                  | 1100                       | 0611                          |                          |                                   |
|         | START          | AA         | 236                                 |                      |                 | 406                                |                      |                 | 483                 |                     |                      |                       | 595                                 |                      |                 | 734                 |                     |                      |                 | ~                   |                     |                      |                            | 778                   | •                | 0001                       | 1000                          |                          |                                   |
|         | CHAIN          | О          | A                                   | -                    |                 | A                                  |                      |                 | A                   | 4                   |                      |                       | A                                   |                      |                 | A                   | ;                   |                      |                 | 4                   | ı.                  |                      |                            | Ą                     |                  | 1                          | 20                            |                          |                                   |
|         | PDB            | А          | 1pam                                |                      |                 | 1pam                               |                      | -               | 1nam                |                     |                      |                       | lpam                                |                      |                 | 1 nam               | - Indi              |                      |                 | 1 nam               | i i                 |                      |                            | 1qq4                  |                  |                            | Idmu                          |                          |                                   |
|         | SEO            | í A Ş      | 1764                                |                      |                 | 1764                               |                      |                 | 1764                | 2                   |                      |                       | 1764                                |                      |                 | 1764                | 10/1                |                      |                 | 1764                |                     |                      |                            | 1764                  |                  |                            | 1764                          |                          |                                   |

|         | PDB annotation |       | CHAPERONE/STRUCTURAL PROTEIN | CHAPERONE/STRUCTURAL PROTEIN CHAPERONE ADHESIN DONOR STRAND COMPLEMENTATION, 2 CHAPERONE/STRUCTURAL PROTEIN                        | CHAPERONE/STRUCTURAL<br>PROTEIN CHAPERONE<br>ADHESIN DONOR STRAND<br>COMPLEMENTATION, 2<br>CHAPERONE/STRUCTURAL<br>PROTEIN         | CHAPERONE/STRUCTURAL PROTEIN CHAPERONE ADHESIN DONOR STRAND COMPLEMENTATION, 2 CHAPERONE/STRUCTURAL PROTEIN                        | CHAPERONE/SIRUCIURAL PROTEIN CHAPERONE ADHESIN DONOR STRAND COMPLEMENTATION, 2 CHAPERONE/STRUCTURAL PROTEIN                        | CHAPERONE/STRUCTURAL PROTEIN CHAPERONE ADHESIN DONOR STRAND COMPLEMENTATION, 2 CHAPERONE/STRUCTURAL                                |
|---------|----------------|-------|------------------------------|------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------|
|         | Compound       |       | P;                           | PAPD-LIKE CHAPERONE FIMC;<br>CHAIN: A, C, E, G, I, K, M, O;<br>MANNOSE-SPECIFIC ADHESIN<br>FIMH; CHAIN: B, D, F, H, J, L, N,<br>P; | PAPD-LIKE CHAPERONE FIMC;<br>CHAIN: A, C, E, G, I, K, M, O;<br>MANNOSE-SPECIFIC ADHESIN<br>FIMH; CHAIN: B, D, F, H, J, L, N,<br>P; | PAPD-LIKE CHAPERONE FIMC;<br>CHAIN: A, C, E, G, I, K, M, O;<br>MANNOSE-SPECIFIC ADHESIN<br>FIMH; CHAIN: B, D, F, H, J, L, N,<br>P; | PAPD-LIKE CHAPERONE FIMC;<br>CHAIN: A, C, E, G, I, K, M, O;<br>MANNOSE-SPECIFIC ADHESIN<br>FIMH; CHAIN: B, D, F, H, J, L, N,<br>P; | PAPD-LIKE CHAPERONE FIMC;<br>CHAIN: A, C, E, G, I, K, M, O;<br>MANNOSE-SPECIFIC ADHESIN<br>FIMH; CHAIN: B, D, F, H, J, L, N,<br>P; |
| Table 5 | SEQ            | Score |                              |                                                                                                                                    |                                                                                                                                    |                                                                                                                                    |                                                                                                                                    |                                                                                                                                    |
| Ta      | PMF            | score |                              | -0.20                                                                                                                              | -0.20                                                                                                                              | -0.20                                                                                                                              | -0.20                                                                                                                              | -0.20                                                                                                                              |
|         | Verify         | score |                              | 0.18                                                                                                                               | 0.26                                                                                                                               | 0.18                                                                                                                               | 0.25                                                                                                                               | 0.08                                                                                                                               |
|         | Psi            | Blast |                              | 8e-33                                                                                                                              | 8e-31                                                                                                                              | 2e-31                                                                                                                              | 1.8e-33                                                                                                                            | 1.4e-14                                                                                                                            |
|         | END            | AA    |                              | 412                                                                                                                                | 320                                                                                                                                | 561                                                                                                                                | 617                                                                                                                                | 179                                                                                                                                |
|         | START          | AA    |                              | 130                                                                                                                                | 16                                                                                                                                 | 242                                                                                                                                | 327                                                                                                                                | 4                                                                                                                                  |
|         | CHAIN          | A     |                              | В                                                                                                                                  | В                                                                                                                                  | В                                                                                                                                  | В                                                                                                                                  | В                                                                                                                                  |
|         | PDB            | А     |                              | 1qun                                                                                                                               | 1qun                                                                                                                               | 1qun                                                                                                                               | 1qun                                                                                                                               | 1qun                                                                                                                               |
|         | SEQ            | ΑŚ    | j.                           | 1764                                                                                                                               | 1764                                                                                                                               | 1764                                                                                                                               | 1764                                                                                                                               | 1764                                                                                                                               |

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|         | PDB annotation |              | PROTEIN | CHAPERONE/STRUCTURAL PROTEIN CHAPERONE                      | ADHESIN DONOR STRAND     | COMPLEMENTATION, 2 CHAPERONE/STRICTIRAL | PROTEIN | CHAPERONE/STRUCTURAL      | PROTEIN CHAPERONE              | ADHESIN DONOR SIRAND     | COMPLEMENTATION, 2                | CHAFEKOINE/SINOCIONAE | PROI EIN | CHAPERONE/STRUCTURAL      | PROTEIN CHAPERONE              | ADHESIN DONOR STRAND     | COMPLEMENTATION, 2                | CHAPERONE/STRUCTURAL | PROTEIN | CHAPERONE/STRUCTURAL      | PROTEIN CHAPERONE              | ADHESIN DONOR STRAND     | COMPLEMENTATION, 2                | CHAPERONE/STRUCTURAL | PROTEIN | CHAPERONE/STRUCTURAL      | PROTEIN CHAPERONE              | ADHESIN DONOR SI KAND    | COMPLEMEN IATION, 2                  | PROTEIN |
|---------|----------------|--------------|---------|-------------------------------------------------------------|--------------------------|-----------------------------------------|---------|---------------------------|--------------------------------|--------------------------|-----------------------------------|-----------------------|----------|---------------------------|--------------------------------|--------------------------|-----------------------------------|----------------------|---------|---------------------------|--------------------------------|--------------------------|-----------------------------------|----------------------|---------|---------------------------|--------------------------------|--------------------------|--------------------------------------|---------|
|         | Compound       |              |         | PAPD-LIKE CHAPERONE FIMC;<br>CHAIN: A. C. E. G. I. K. M. O; | MANNOSE-SPECIFIC ADHESIN | FIMH; CHAIN: B, D, F, H, J, L, N,       | .,      | PAPD-LIKE CHAPERONE FIMC; | CHAIN: A, C, E, G, I, K, M, O; | MANNOSE-SPECIFIC ADHESIN | FIMH; CHAIN: B, D, F, H, J, L, N, | <del>.</del>          |          | PAPD-LIKE CHAPERONE FIMC; | CHAIN: A, C, E, G, I, K, M, O; | MANNOSE-SPECIFIC ADHESIN | FIMH; CHAIN: B, D, F, H, J, L, N, | ò                    |         | PAPD-LIKE CHAPERONE FIMC; | CHAIN: A, C, E, G, I, K, M, O; | MANNOSE-SPECIFIC ADHESIN | FIMH; CHAIN: B, D, F, H, J, L, N, | P;                   |         | PAPD-LIKE CHAPERONE FIMC; | CHAIN: A, C, E, G, I, K, M, O; | MANNOSE-SPECIFIC ADHESIN | FIMH; CHAIN: B, D, F, H, J, L, N, P. | Г,      |
| Table 5 | SEQ            | FOLD         |         |                                                             |                          |                                         |         |                           |                                |                          |                                   |                       |          |                           |                                |                          |                                   |                      |         |                           |                                |                          |                                   |                      |         |                           |                                |                          |                                      |         |
| Tab     | PMF            | score        |         | -0.20                                                       |                          |                                         |         | -0.20                     |                                |                          |                                   |                       |          | 0.70                      |                                |                          |                                   |                      |         | -0.20                     |                                |                          |                                   |                      |         | -0.18                     |                                |                          |                                      |         |
|         | Verify         | score        |         | 0.34                                                        | -                        |                                         |         | 0.24                      |                                |                          |                                   |                       |          | 0.17                      |                                |                          |                                   |                      |         | 0.21                      |                                |                          |                                   |                      |         | 0.26                      |                                |                          |                                      |         |
| İ       | Psi            | Blast        |         | 2e-32                                                       |                          |                                         |         | 1e-35                     |                                |                          |                                   |                       |          | 2e-30                     |                                |                          |                                   |                      |         | 4e-30                     |                                |                          |                                   |                      |         | 1e-31                     |                                |                          |                                      |         |
|         | END            | AA           |         | 669                                                         |                          |                                         |         | 764                       |                                |                          |                                   |                       |          | 988                       |                                |                          |                                   |                      |         | 943                       | <u> </u>                       |                          |                                   |                      |         | 1012                      |                                |                          |                                      |         |
|         | START          | AA           |         | 418                                                         |                          |                                         |         | 464                       | 2                              |                          |                                   |                       |          | 009                       |                                |                          |                                   |                      |         | 654                       | -                              |                          |                                   |                      |         | 721                       |                                |                          |                                      |         |
|         | CHAIN          | <u></u><br>요 |         | В                                                           |                          |                                         |         | ď                         |                                |                          |                                   |                       |          | B                         | 1                              |                          |                                   |                      |         | a                         | à.                             |                          |                                   |                      |         | В                         |                                |                          |                                      |         |
|         | PDB            | <u> </u>     |         | 1dnm                                                        |                          |                                         |         | 101                       | ımbı                           |                          |                                   |                       |          | lann                      | ļ,                             | •                        |                                   |                      |         | 101111                    | Imbr                           |                          |                                   |                      |         | 10un                      |                                |                          |                                      |         |
|         | SEQ            | ВŞ           |         | 1764                                                        |                          |                                         |         | 1764                      |                                |                          | -                                 |                       |          | 1764                      |                                |                          |                                   |                      |         | 1761                      | <br>t<br>0/1                   |                          |                                   |                      |         | 1764                      |                                |                          |                                      |         |

|         |                      |                                                                                         |                                                       |                                                                                         |                                                       |                                                             |                          |                              |                           |                          |                                   |                                 |                                        |                          |                                   |                                 | $\overline{}$            |
|---------|----------------------|-----------------------------------------------------------------------------------------|-------------------------------------------------------|-----------------------------------------------------------------------------------------|-------------------------------------------------------|-------------------------------------------------------------|--------------------------|------------------------------|---------------------------|--------------------------|-----------------------------------|---------------------------------|----------------------------------------|--------------------------|-----------------------------------|---------------------------------|--------------------------|
|         | PDB annotation       | CHAPERONE/STRUCTURAL<br>PROTEIN CHAPERONE<br>ADHESIN DONOR STRAND                       | COMPLEMENTATION, 2<br>CHAPERONE/STRUCTURAL<br>PROTEIN | CHAPERONE/STRUCTURAL<br>PROTEIN CHAPERONE<br>ADHESIN DONOR STRAND                       | COMPLEMENTATION, 2<br>CHAPERONE/STRUCTURAL<br>PROTEIN | CHAPERONE/STRUCTURAL PROTEIN CHAPERONE                      | ADHESIN DONOR STRAND     | CHAPERONE/STRUCTURAL PROTEIN | CHAPERONE/STRUCTURAL      | ADHESIN DONOR STRAND     | COMPLEMENTATION, 2                | CHAPEKUNE/SIKUCIUKAL<br>PROTEIN | CHAPERONE/STRUCTURAL PROTEIN CHAPERONE | ADHESIN DONOR STRAND     | COMPLEMENTATION, 2                | CHAPERONE/STRUCTURAL<br>PROTEIN |                          |
|         | Compound             | PAPD-LIKE CHAPERONE FIMC;<br>CHAIN: A, C, E, G, I, K, M, O;<br>MANNOSE-SPECIFIC ADHESIN | FIMH; CHAIN: B, D, F, H, J, L, N, P;                  | PAPD-LIKE CHAPERONE FIMC;<br>CHAIN: A, C, E, G, I, K, M, O;<br>MANNOSE-SPECIFIC ADHESIN | FIMH; CHAIN: B, D, F, H, J, L, N, P;                  | PAPD-LIKE CHAPERONE FIMC;<br>CHAIN: A, C, E, G, I, K, M, O; | MANNOSE-SPECIFIC ADHESIN | P;                           | PAPD-LIKE CHAPERONE FIMC; | MANNOSE-SPECIFIC ADHESIN | FIMH; CHAIN: B, D, F, H, J, L, N, | P;                              | PAPD-LIKE CHAPERONE FIMC;              | MANNOSE-SPECIFIC ADHESIN | FIMH; CHAIN: B, D, F, H, J, L, N, | p,                              | VIRUS TOMATO BUSHY STUNT |
| Table 5 | SEQ<br>FOLD<br>score |                                                                                         |                                                       |                                                                                         |                                                       |                                                             |                          |                              |                           |                          |                                   |                                 |                                        |                          |                                   |                                 |                          |
| Tab     | PMF                  | -0.20                                                                                   |                                                       | -0.19                                                                                   |                                                       | -0.19                                                       |                          |                              | -0.19                     |                          |                                   |                                 | -0.20                                  |                          |                                   |                                 | -0.20                    |
|         | Verify<br>score      | 0.27                                                                                    |                                                       | 0.22                                                                                    |                                                       | 0.34                                                        |                          |                              | 0.25                      |                          |                                   |                                 | 0.16                                   |                          |                                   |                                 | 0.11                     |
|         | Psi<br>Blast         | 8e-32                                                                                   |                                                       | 4e-34                                                                                   |                                                       | 8e-33                                                       |                          |                              | 1e-33                     |                          |                                   |                                 | 4e-21                                  |                          |                                   |                                 | 8e-34                    |
|         | END                  | 358                                                                                     |                                                       | 1051                                                                                    |                                                       | 1127                                                        |                          |                              | 1164                      |                          |                                   |                                 | 1183                                   |                          |                                   |                                 | 340                      |
|         | START<br>AA          | 74                                                                                      |                                                       | 765                                                                                     |                                                       | 821                                                         |                          |                              | 901                       |                          |                                   |                                 | 996                                    |                          |                                   |                                 | 18                       |
|         | CHAIN                | В                                                                                       |                                                       | В                                                                                       |                                                       | В                                                           |                          |                              | В                         |                          |                                   |                                 | В                                      |                          |                                   |                                 | C                        |
|         | PDB<br>ID            | 1qun                                                                                    |                                                       | 1qun                                                                                    |                                                       | 1qun                                                        |                          |                              | 1qun                      |                          |                                   |                                 | 1qun                                   |                          |                                   |                                 | 2tbv                     |
|         | SEQ<br>EQ            | 1764                                                                                    |                                                       | 1764                                                                                    |                                                       | 1764                                                        |                          |                              | 1764                      |                          |                                   |                                 | 1764                                   |                          |                                   |                                 | 1764                     |

|         |                |       |       | т-           | Τ                        |              |                          |                           |              |                          |              |                                          | _ |        |                                          |                        |                              |                                   |                     |                     |             |                         |                           | -                    |        | <del></del>              |                            |                    |                       |         | _                        |                                          |
|---------|----------------|-------|-------|--------------|--------------------------|--------------|--------------------------|---------------------------|--------------|--------------------------|--------------|------------------------------------------|---|--------|------------------------------------------|------------------------|------------------------------|-----------------------------------|---------------------|---------------------|-------------|-------------------------|---------------------------|----------------------|--------|--------------------------|----------------------------|--------------------|-----------------------|---------|--------------------------|------------------------------------------|
|         | PDB annotation |       |       |              |                          |              |                          |                           |              |                          |              |                                          |   |        | SIGNALING PROTEIN                        | FACTELIN-LIGAIND       | DECOCATTION DETAILME         | AECOGINITION, BELA LUKIN          | SIGNALING PROTEIN   | PLECKSTRIN HOMOLOGY | DOMAIN FOLD | SIGNALING PROTEIN VASP; | EVH1, VASP-ENA, NMR,      | POLY-PROLINE-BINDING | DOMAIN | CONTRACTILE PROTEIN      | WH1 DOMAIN; MOLECULAR      | RECOGNITION, ACTIN | DYNAMICS, CONTRACTILE | PROTEIN | CONTRACTILE PROTEIN      | WHI DOMAIN; MOLECULAR RECOGNITION, ACTIN |
|         | Compound       |       |       | VIRUS 2TBV 4 | VIRUS TOMATO BUSHY STUNT | VIRUS ZIBV 4 | VIRUS TOMATO BUSHY STUNT | VIRIS TOMATO BUSIN STRING | VIRUS 2TBV 4 | VIRUS TOMATO BUSHY STUNT | VIRUS 2TBV 4 | VIRUS TOMATO BUSHY STUNT<br>VIRUS 2TBV 4 |   |        | GLGF-DOMAIN PROTEIN<br>HOMFR : CHAIN: A: | METABOTRODIC GITTANATE | RECEPTOR MGI 11R5: CHAIN: B. | OI OF FOR CHANGE ONLY, CALMEN, D, | GLGF-DOMAIN PROTEIN | HOMEK; CHAIN: A;    |             | VASODILATOR-STIMULATED  | PHOSPHOPROTEIN; CHAIN: A; |                      |        | MENA EVH1 DOMAIN; CHAIN: | A; PEPTIDE ACTA; CHAIN: B; |                    |                       |         | MENA EVH1 DOMAIN; CHAIN: | A; PEPTIDE ACTA; CHAIN: B;               |
| Table 5 | SEQ            | FOLD  | score |              |                          |              |                          |                           |              |                          |              |                                          |   |        |                                          |                        |                              |                                   |                     |                     |             |                         |                           |                      |        | 83.11                    |                            |                    |                       |         |                          |                                          |
| T       | PMF            | score |       |              | -0.20                    | 6            | 07:0-                    | -0.20                     | 1            | -0.20                    |              | -0.20                                    |   | 000    | V.59                                     |                        |                              | 700                               | 0.04                |                     |             | T:00                    |                           |                      |        |                          |                            |                    |                       |         | 1.00                     |                                          |
|         | Verify         | score |       |              | 0.19                     | 000          | 67.0                     | 0.19                      | N<br>I       | 0.25                     |              | 0.19                                     |   | 0.00   | CC:0                                     |                        |                              | 0.70                              | 6/:0                |                     |             | 0.94                    |                           |                      |        |                          |                            |                    |                       |         | 0.93                     |                                          |
|         | Psi            | Blast |       |              | 1.8e-34                  | 1 10.26      | 1.46-50                  | 4e-38                     |              | 6e-34                    |              | 4e-35                                    |   | 600 77 | 0.95-27                                  | -                      |                              | 6 80 30                           | 0.00.0              |                     | 10.00       | 1.26-30                 |                           |                      | 000    | 6.8e-38                  |                            |                    |                       | 0       | 0.8e-38                  |                                          |
|         | END:           | AA    |       | !            | 643                      | 775          |                          | 995                       |              | 1166                     |              | 441                                      |   | 121    | 171                                      |                        |                              | 122                               | 777                 | ,                   | 127         | <del>1</del> 77         | _                         | •                    | ,      | 771                      |                            | _                  |                       |         | 771                      |                                          |
|         | START          | AA    |       | 100          | 307                      | 447          | Ĩ                        | 199                       |              | 836                      |              | 68                                       |   | 13     | 2                                        |                        |                              | 8                                 | )                   |                     | 0           | 0                       |                           |                      | 0      | <u>ب</u>                 |                            |                    | •                     |         | 7                        |                                          |
|         | CHAIN          | 3     |       |              | <u>-</u>                 | C            | )                        | S                         |              | ပ                        |              | ပ                                        |   | A      | •                                        |                        |                              | \<br>\                            |                     |                     | V           | 17                      |                           |                      |        | ¥.                       |                            |                    |                       |         | τ                        |                                          |
| 444     | FUB<br>TI      | 1     |       | 170          | AQ17                     | 2fbv         |                          | 2tbv                      |              | 2tbv                     | 1            | Ztbv                                     |   | 1 ddv  |                                          |                        |                              | 1ddw                              |                     | _                   | 1 pay       | , a                     |                           |                      | 1 ovh  | ICAII                    |                            |                    |                       | 1 orth  | Tevil                    |                                          |
| 5       | SEC<br>1       | g g   |       | 1761         | 1/04                     | 1764         |                          | 1764                      |              | 1764                     | 1725         | 1/04                                     |   | 1769   |                                          |                        |                              | 1769                              |                     |                     | 1769        | <u> </u>                |                           |                      | 1760   |                          |                            |                    |                       | 1760    |                          |                                          |

|         | PDB annotation       | DYNAMICS, CONTRACTILE PROTEIN | CELL MOTILITY AN INCOMPLETE SEVEN STRANDED ANTI-PARALLEL BETA BARREL 2 CLOSED BY AN ALPHA HELIX, EVHI DOMAIN, ACTIN-BASED CELL 3 MOTILITY, INTERACTION MODULE | CELL MOTILITY AN INCOMPLETE SEVEN STRANDED ANTI- PARALLEI. BETA BARREL 2 CLOSED BY AN ALPHA HELIX, EVHI DOMAIN, ACTIN-BASED CELL 3 MOTILITY, INTERACTION MODULE |                                                                                  |                                                                                 | COMPLEX<br>(INHIBITOR/NUCLEASE)<br>COMPLEX                          |
|---------|----------------------|-------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------|---------------------------------------------------------------------------------|---------------------------------------------------------------------|
|         | Compound             |                               | EVHI DOMAIN FROM ENA/VASP-LIKE PROTEIN; CHAIN: A, B; PHE-GLU-PHE- PRO-PRO-PRO-THR-ASP- GLU-GLU; CHAIN: C, D;                                                  | EVH1 DOMAIN FROM ENA/VASP-LIKE PROTEIN; CHAIN: A, B; PHE-GLU-PHE- PRO-PRO-PRO-THR-ASP- GLU-GLU; CHAIN: C, D;                                                    | OXIDOREDUCTASE(OXYGEN(A)<br>) GALACTOSE OXIDASE<br>(E.C.1.1.3.9) (PH 4.5) 1GOF 3 | OXIDOREDUCTASE(OXYGEN(A))<br>GALACTOSE OXIDASE<br>(E.C.1.1.3.9) (PH 4.5) 1GOF 3 | RIBONUCLEASE INHIBITOR;<br>CHAIN: A, D; ANGIOGENIN;<br>CHAIN: B, E; |
| Table 5 | SEQ<br>FOLD<br>score |                               |                                                                                                                                                               | 62.45                                                                                                                                                           |                                                                                  |                                                                                 |                                                                     |
| Tab     | PMF<br>score         |                               | 1.00                                                                                                                                                          |                                                                                                                                                                 | 0.23                                                                             | 0.16                                                                            | 0.23                                                                |
|         | Verify<br>score      |                               | 0.93                                                                                                                                                          |                                                                                                                                                                 | -0.16                                                                            | 0.03                                                                            | -0.25                                                               |
|         | Psi<br>Blast         |                               | 1.7e-32                                                                                                                                                       | 1.7e-32                                                                                                                                                         | 8e-23                                                                            | 0.0041                                                                          | 4e-16                                                               |
|         | END                  |                               | 119                                                                                                                                                           | 121                                                                                                                                                             | 449                                                                              | 450                                                                             | 154                                                                 |
|         | START                |                               | ∞                                                                                                                                                             | 6                                                                                                                                                               | 183                                                                              | 344                                                                             | 6                                                                   |
|         | CHAIN<br>ID          |                               | A                                                                                                                                                             | 4                                                                                                                                                               |                                                                                  |                                                                                 | A                                                                   |
|         | PDB<br>ID            |                               | 19c6                                                                                                                                                          | 14c6                                                                                                                                                            | 1gof                                                                             | 1gof                                                                            | 1a4y                                                                |
|         | SEQ<br>ID            |                               | 1769                                                                                                                                                          | 1769                                                                                                                                                            | 1772                                                                             | 1772                                                                            | 1775                                                                |

Table 5

|         |                |            |                                            |                       |                      |                                    |                              |                               |                                |                        | _  |                                                                               |     |                        |                                 |                                                                               |      |                           |                              |                                                  |     |                        |                        |                              |
|---------|----------------|------------|--------------------------------------------|-----------------------|----------------------|------------------------------------|------------------------------|-------------------------------|--------------------------------|------------------------|----|-------------------------------------------------------------------------------|-----|------------------------|---------------------------------|-------------------------------------------------------------------------------|------|---------------------------|------------------------------|--------------------------------------------------|-----|------------------------|------------------------|------------------------------|
|         | PDB annotation |            | (INHIBITOR/NUCLEASE),<br>COMPLEX (RI-ANG), | HYDROLASE 2 MOLECULAR | RECOGNITION, EPITOPE | MAPPING, LEUCINE-RICH 3<br>REPEATS | COMPLEX (NUCLEAR             | PROTEIN/RNA) COMPLEX          | (NUCLEAK PKOTEIN/KINA),<br>PNA | SNRNP, RIBONUCLEOPROTE | Z. | COMPLEX (NUCLEAR PROTEIN/RNA) (NUCLEAR PROTEIN/RNA),                          | RNA | SNRNP, RIBONUCLEOPROTE | COMPLEY (MITCHEAR               | PROTEIN/RNA) COMPLEX (NUCLEAR PROTEIN/RNA),                                   | RNA, | SNRNP, RIBONUCLEOPROTE IN | COMPLEX (NUCLEAR             | PROTEIN/RNA) COMPLEX<br>  (NUCLEAR PROTEIN/RNA), | RNA | SNRNP, RIBONUCLEOPROTE | IN CONTROLLY OF THE AT | COMPLEX (NUCLEAR             |
|         | Compound       |            |                                            |                       |                      |                                    | U2 RNA HAIRPIN IV; CHAIN: Q, | R; U2 A'; CHAIN: A, C; U2 B"; | CHAIN: B, D;                   |                        |    | U2 RNA HAIRPIN IV; CHAIN: Q,<br>R; U2 A'; CHAIN: A, C; U2 B";<br>CHAIN: R. D. |     |                        | TO DOLL WE WANTED IN CITABLE OF | UZ KNA HAIKTIN IV; CHAIN: Q,<br>R; UZ A'; CHAIN: A, C; UZ B";<br>CHAIN: B. D: |      |                           | U2 RNA HAIRPIN IV; CHAIN: Q, | R; U2 A'; CHAIN: A, C; U2 B";<br>CHAIN: B D:     |     |                        |                        | U2 RNA HAIRPIN IV; CHAIN: Q, |
| Table 5 | SEQ            | FOLD score |                                            |                       | -                    |                                    |                              |                               |                                |                        |    |                                                                               |     |                        |                                 |                                                                               |      |                           |                              |                                                  |     |                        |                        |                              |
| Tab     | PMF            | score      |                                            |                       |                      |                                    | 0.16                         | )                             |                                |                        |    | 69.0                                                                          |     |                        | ,                               | 1.00                                                                          |      |                           | 0.76                         |                                                  |     |                        |                        | 0.47                         |
|         | Verify         | score      |                                            |                       |                      |                                    | -0.28                        |                               |                                |                        |    | 0.20                                                                          |     |                        |                                 | 0.67                                                                          |      |                           | 0.42                         |                                                  |     |                        |                        | -0.10                        |
|         | Psi            | Blast      |                                            |                       |                      |                                    | 16-08                        | 3                             |                                |                        |    | 1e-09                                                                         |     |                        |                                 | 4e-22                                                                         |      |                           | 2e-20                        |                                                  |     |                        |                        | 1.2e-08                      |
|         | END            | ΑA         |                                            |                       |                      |                                    | 105                          |                               |                                |                        |    | 107                                                                           |     |                        |                                 | 169                                                                           |      |                           | 122                          |                                                  |     |                        |                        | 195                          |
|         | START          | AA         |                                            |                       |                      |                                    | 126                          | 071                           |                                |                        |    | 3                                                                             |     |                        |                                 | 32                                                                            |      |                           | 2                            | 1                                                |     |                        |                        | 126                          |
|         | CHAIN          | <u> </u>   |                                            |                       |                      | ***                                |                              | €                             |                                |                        |    | А                                                                             |     |                        |                                 | Ą                                                                             |      |                           | A                            | <b>.</b>                                         |     |                        |                        | S                            |
|         | PDB            | <u>a</u>   |                                            |                       |                      | -1                                 | 1001                         | 12911                         |                                |                        |    | la9n                                                                          |     |                        |                                 | 1a9n                                                                          |      |                           | 1a9n                         | 14011                                            |     |                        |                        | la9n                         |
|         | SEQ            | 日 Ş        | <br>                                       |                       |                      |                                    | 1775                         | C//I                          |                                |                        |    | 1775                                                                          |     |                        |                                 | 1775                                                                          | _    |                           | 1775                         |                                                  |     |                        |                        | 1775                         |

|         | PDB annotation       | PROTEINRNA) COMPLEX<br>(NUCLEAR PROTEINRNA),<br>RNA,<br>SNRNP, RIBONUCLEOPROTE | IN<br>COMPLEX (NUCLEAR<br>PROTEIN/RNA) COMPLEX<br>(NUCLEAR PROTEIN/RNA),<br>RNA,<br>SNRNP,RIBONUCLEOPROTE | COMPLEX (NUCLEAR PROTEIN/RNA) COMPLEX (NUCLEAR PROTEIN/RNA), RNA, SNRNP, RIBONUCLEOPROTE | COMPLEX (NUCLEAR<br>PROTEIN/RNA) COMPLEX<br>(NUCLEAR PROTEIN/RNA),<br>RNA,<br>SNRNP, RIBONUCLEOPROTE<br>IN | CELL ADHESION LEUCINE<br>RICH REPEAT, CALCIUM<br>BINDING, CELL ADHESION | CELL ADHESION LEUCINE<br>RICH REPEAT, CALCIUM<br>BINDING, CELL ADHESION | CELL ADHESION LEUCINE<br>RICH REPEAT, CALCIUM |
|---------|----------------------|--------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------|-------------------------------------------------------------------------|-----------------------------------------------|
|         | Compound             | R; U2 A'; CHAIN: A, C; U2 B";<br>CHAIN: B, D;                                  | U2 RNA HAIRPIN IV; CHAIN: Q,<br>R; U2 A'; CHAIN: A, C; U2 B";<br>CHAIN: B, D;                             | U2 RNA HAIRPIN IV; CHAIN: Q,<br>R; U2 A'; CHAIN: A, C; U2 B";<br>CHAIN: B, D;            | U2 RNA HAIRPIN IV; CHAIN: Q,<br>R; U2 A'; CHAIN: A, C; U2 B";<br>CHAIN: B, D;                              | INTERNALIN B; CHAIN: A;                                                 | INTERNALIN B; CHAIN: A;                                                 | INTERNALIN B; CHAIN: A;                       |
| Table 5 | SEQ<br>FOLD<br>score |                                                                                |                                                                                                           |                                                                                          |                                                                                                            |                                                                         |                                                                         |                                               |
| Tab     | PMF<br>score         |                                                                                | 0.87                                                                                                      | 0.93                                                                                     | 0.88                                                                                                       | 1.00                                                                    | 1.00                                                                    | 0.75                                          |
|         | Verify               |                                                                                | 0.37                                                                                                      | 0.37                                                                                     | 0.50                                                                                                       | 0.65                                                                    | 0.22                                                                    | 0.05                                          |
|         | Psi<br>Blast         |                                                                                | 1e-09                                                                                                     | 8e-23                                                                                    | 2e-20                                                                                                      | 1e-26                                                                   | 5.1e-28                                                                 | 1.4e-20                                       |
|         | END                  |                                                                                | 107                                                                                                       | 169                                                                                      | 122                                                                                                        | 128                                                                     | 192                                                                     | 238                                           |
|         | START                |                                                                                | 23                                                                                                        | 32                                                                                       | v.                                                                                                         | -                                                                       | 21                                                                      | 47                                            |
|         | CHAIN                |                                                                                | U                                                                                                         | U                                                                                        | v                                                                                                          | A                                                                       | A                                                                       | A                                             |
|         | PDB<br>ID            |                                                                                | 1a9n                                                                                                      | 1a9n                                                                                     | 1a9n                                                                                                       | 1d0b                                                                    | 1d0b                                                                    | 1d0b                                          |
|         | SEQ<br>FD            | O                                                                              | 1775                                                                                                      | 1775                                                                                     | 1775                                                                                                       | 1775                                                                    | 1775                                                                    | 1775                                          |

|         | PDB annotation |       |
|---------|----------------|-------|
|         | Compound       |       |
| Table 5 | SEQ<br>FOLD    | score |
| Ta      | PMF<br>score   |       |
|         | Verify         |       |
|         | Psi<br>Blast   |       |
|         | END            |       |
|         | START          |       |
|         | CHAIN          |       |
|         | DB             | }     |

|          | PDB annotation  | BINDING, CELL ADHESION | CELL ADHESION LEUCINE RICH REPEAT, CALCIUM BINDING, CELL ADHESION | TRANSFERASE CRYSTAL | STRUCTURE, RAB         | GEKAN Y LGEKAN Y LI KANSF<br>ERASE, 2.0 A 2 | RESOLUTION, N-         | FORMYLMETHIONINE,           | ALPHA SUBUNIT, BETA<br>SUBUNIT | TRANSFERASE CRYSTAL | STRUCTURE, RAB         | GERANYLGERANYLIKANSF      | ERASE, 2.0 A 2 | RESOLUTION, N-         | FORMYLMEIHIONINE,           | ALPHA SUBUNIT, BETA | SUBUNII | IKANSFEKASE CKISIAL | STRUCTURE, RAB         | GERANYLGERANYLTRANSF      | ERASE, 2.0 A 2 | RESOLUTION, N-         | FORMYI METHIONINE.           | ALPHA SUBUNIT. BETA | SUBUNIT | TRANSFERASE CRYSTAL | STRUCTURE, RAB         | GENALI DOLINGIA LELIGIANIA |
|----------|-----------------|------------------------|-------------------------------------------------------------------|---------------------|------------------------|---------------------------------------------|------------------------|-----------------------------|--------------------------------|---------------------|------------------------|---------------------------|----------------|------------------------|-----------------------------|---------------------|---------|---------------------|------------------------|---------------------------|----------------|------------------------|------------------------------|---------------------|---------|---------------------|------------------------|----------------------------|
|          | Compound        |                        | INTERNALIN B; CHAIN: A;                                           | RAB                 | GERANYLGERANYLTRANSFER | ASE ALPHA SUBUNIT; CHAIN:<br>A. C; RAB      | GERANYLGERANYLTRANSFER | ASE BETA SUBUNIT; CHAIN: B, | D;                             | RAB                 | GERANYLGERANYLTRANSFER | ASE ALPHA SUBUNIT; CHAIN: | A, C; RAB      | GERANYLGERANYLTRANSFER | ASE BETA SUBUNIT; CHAIN: B, | D;                  |         | RAB                 | GERANYLGERANYLTRANSFER | ASE ALPHA SUBUNIT; CHAIN: | A. C. RAB      | GERANYLGERANYLTRANSFER | ASE BETA STIBITUIT: CHAIN: B | D.                  | ŗ.      | RAB                 | GERANYLGERANYLTRANSFER | ASE ALPHA SUBUNII; CHAIN:  |
| Table 5  | SEQ<br>FOLD     | 200                    |                                                                   |                     | •                      |                                             |                        |                             |                                |                     |                        |                           |                |                        |                             |                     |         |                     |                        |                           |                |                        |                              |                     |         |                     |                        |                            |
| Ta<br>Ta | PMF<br>score    |                        | 0.70                                                              | 0.03                | C.Y.V                  |                                             |                        |                             |                                | 86.0                | )<br>}                 |                           |                |                        |                             |                     |         | 0.93                |                        |                           |                |                        |                              |                     |         | 0 11                | •                      |                            |
|          | Verify<br>score |                        | 0.18                                                              | 0.13                | -0.13                  |                                             |                        |                             |                                | 0.32                | 1                      |                           |                |                        |                             |                     |         | 0.62                |                        |                           |                |                        |                              |                     |         | 0.30                |                        |                            |
|          | Psi<br>Blast    |                        | 4e-31                                                             | 170 11              | 1./6-11                |                                             |                        |                             |                                | 1 70-13             | 1:72                   |                           |                |                        |                             |                     |         | 1.2e-15             |                        |                           |                |                        |                              |                     |         | 2 10 11             |                        |                            |
|          | END<br>AA       |                        | 197                                                               | 107                 | 197                    |                                             |                        |                             |                                | 128                 | 071                    |                           |                |                        |                             |                     |         | 106                 |                        |                           |                |                        |                              |                     | -       | 107                 | <u></u>                |                            |
|          | START<br>AA     |                        | ∞                                                                 | 144                 | 144<br>1               |                                             |                        |                             |                                | 23                  | 7                      |                           |                |                        |                             |                     |         | 5                   |                        |                           |                |                        |                              |                     |         | 1/4                 | <u>t</u>               |                            |
|          | CHAIN           |                        | A                                                                 |                     | A                      |                                             |                        |                             |                                | <                   | ¥.                     |                           |                |                        |                             |                     |         | A                   |                        |                           |                |                        |                              |                     |         |                     | ۲                      |                            |
|          | PDB<br>ID       |                        | 1d0b                                                              | -                   | l dce                  |                                             |                        |                             |                                | 1900                | agn                    |                           |                |                        |                             |                     |         | 1dce                |                        |                           |                |                        |                              |                     |         | 1.1                 | Jace                   |                            |
|          | SEQ             | NO:                    | 1775                                                              |                     | 1775                   |                                             |                        |                             |                                | 3771                | C//I                   |                           |                |                        |                             |                     | ,,,,    | 1775                | ,°                     |                           |                |                        |                              |                     |         | 1                   | 0//1                   |                            |

|         | PDB annotation  | ERASE, 2.0 A 2 RESOLUTION, N-FORMYLMETHIONINE,              | ALPHA SUBUNII, BEIA<br>SUBUNIT | CONTRACTILE PROTEIN                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           | BETA-BETA-ALPHA<br>CYLINDER, DYNEIN, 2 | CHLAMYDOMONAS,<br>FLAGELLA | CONTRACTILE PROTEIN           | LEUCINE-RICH REPEAT, | BETA-BETA-ALPHA | CHLAMYDOMONAS, | FLAGELLA | RNA BINDING PROTEIN TAP | (NFX1);                | RIBONUCLEOPROTEIN | (KNP,KBD OK KKM) AND | LEUCINE-KICH-KEFEA1 2 (TRR) | RNA BINDING PROTEIN TAP | (NFX1); | RIBONUCLEOPROTEIN | (RNP,RBD OR RRM) AND | LEUCINE-RICH-REPEAT 2 | (LRR) | LIGASE CYCLIN A/CDK2-<br>ASSOCIATED PROTEIN P45;                    |
|---------|-----------------|-------------------------------------------------------------|--------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------|----------------------------|-------------------------------|----------------------|-----------------|----------------|----------|-------------------------|------------------------|-------------------|----------------------|-----------------------------|-------------------------|---------|-------------------|----------------------|-----------------------|-------|---------------------------------------------------------------------|
|         | Compound        | C; RAB<br>RANYLGERANYLTRANSFER<br>E BETA SUBUNIT; CHAIN: B, |                                | OUTER ARM DYNEIN; CHAIN: A; CUTER ARM DYNEIN; CHAIN: A; | H O                                    | O H                        | OUTER ARM DYNEIN; CHAIN: A; C | 1                    | T C             |                | 144      | NUCLEAR RNA EXPORT F    | FACTOR 1; CHAIN: A, B; |                   |                      |                             | NIJCLEAR RNA EXPORT     |         |                   |                      |                       |       | SKP2; CHAIN: A, C, E, G, I, K, M, O; SKP1; CHAIN: B, D, F, H, I, L, |
| Table 5 | SEQ<br>FOLD     | 21026                                                       |                                |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |                                        |                            |                               |                      |                 |                |          |                         |                        |                   |                      |                             |                         |         |                   |                      |                       |       |                                                                     |
| Tab     | PMF<br>score    |                                                             |                                | 0.11                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          | -1                                     |                            | 0.18                          |                      |                 |                |          | 0.58                    |                        |                   |                      |                             | 0.37                    |         |                   |                      |                       |       | 0.25                                                                |
|         | Verify<br>score |                                                             |                                | -0.37                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |                                        |                            | -0.65                         |                      |                 |                |          | 0.25                    |                        |                   |                      |                             | -0.78                   | ?       |                   |                      |                       |       | 0.09                                                                |
|         | Psi<br>Blast    |                                                             |                                | 5.1e-16                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |                                        | -                          | 5.1e-17                       |                      |                 |                |          | 1.7e-07                 |                        |                   |                      |                             | 3 40-06                 | 00-24-5 |                   |                      |                       |       | 1e-09                                                               |
|         | END             |                                                             |                                | 106                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |                                        |                            | 197                           |                      |                 |                |          | 123                     | 1                      |                   |                      |                             | 107                     | 121     |                   |                      |                       |       | 193                                                                 |
|         | START<br>AA     |                                                             |                                |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |                                        |                            | 83                            | )                    |                 |                |          | 46                      | 2                      |                   |                      |                             | 145                     | £1      |                   |                      |                       |       | 51                                                                  |
|         | CHAIN           |                                                             |                                | A                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |                                        |                            | 4                             | 47                   |                 |                |          | A                       |                        |                   |                      |                             | £                       | q       |                   | ÷                    |                       |       | А                                                                   |
|         | PDB<br>ID       |                                                             |                                | 1ds9                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |                                        | _                          | 1460                          | ) con                |                 |                |          | 1 fo 1                  |                        |                   |                      |                             | 1.62.1                  | 1011    |                   |                      |                       |       | 1fqv                                                                |
|         | SEQ             | <br>OZ                                                      |                                | 1775                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |                                        |                            | 1775                          |                      |                 |                |          | 1775                    |                        |                   |                      |                             | 1776                    | C//I    |                   |                      |                       |       | 1775                                                                |

|         | PDB annotation       | CYCLIN A/CDK2-<br>ASSOCIATED PROTEIN P19;<br>SKP1, SKP2, F-BOX, LRR,<br>LEUCINE-RICH REPEAT,<br>SCF, UBIQUITIN, 2 E3,<br>UBIQUITIN PROTEIN<br>LIGASE | LIGASE CYCLIN A/CDK2-<br>ASSOCIATED P45; CYCLIN<br>A/CDK2-ASSOCIATED P19;<br>SKP1, SKP2, F-BOX, LRRS,<br>LEUCINE-RICH REPEATS,<br>SCF, 2 UBIQUITIN, E3,<br>UBIQUITIN PROTEIN<br>LIGASE | LIGASE CYCLIN A/CDK2-<br>ASSOCIATED P45; CYCLIN<br>A/CDK2-ASSOCIATED P19;<br>SKP1, SKP2, F-BOX, LRRS,<br>LEUCINE-RICH REPEATS,<br>SCF, 2 UBIQUITIN, E3,<br>UBIQUITIN PROTEIN<br>LIGASE | TRANSCRIPTION RNAIP; RANGAP; GTPASE- ACTIVATING PROTEIN FOR SPI1, GTPASE-ACTIVATING PROTEIN, GAP, RNAIP, RANGAP, LRR, LEUCINE- 2 RICH REPEAT PROTEIN, TWINNING, HEMIHEDRAL |
|---------|----------------------|------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
|         | Compound             | N, P;                                                                                                                                                | SKP2; CHAIN: A, C; SKP1;<br>CHAIN: B, D;                                                                                                                                               | SKP2; CHAIN: A, C; SKP1;<br>CHAIN: B, D;                                                                                                                                               | GTPASE-ACTIVATING PROTEIN<br>RNA1_SCHPO; CHAIN: A, B;                                                                                                                      |
| Table 5 | SEQ<br>FOLD<br>score |                                                                                                                                                      |                                                                                                                                                                                        |                                                                                                                                                                                        |                                                                                                                                                                            |
| Tal     | PMF<br>score         |                                                                                                                                                      | 0.75                                                                                                                                                                                   | 0.33                                                                                                                                                                                   | 0.37                                                                                                                                                                       |
|         | Verify<br>score      |                                                                                                                                                      | -0.05                                                                                                                                                                                  | -0.11                                                                                                                                                                                  | 0.02                                                                                                                                                                       |
|         | Psi<br>Blast         |                                                                                                                                                      | 2e-22                                                                                                                                                                                  | 1e-09                                                                                                                                                                                  | 2e-20                                                                                                                                                                      |
|         | END                  |                                                                                                                                                      | 189                                                                                                                                                                                    | 193                                                                                                                                                                                    | 196                                                                                                                                                                        |
|         | START<br>AA          |                                                                                                                                                      | 80                                                                                                                                                                                     | 51                                                                                                                                                                                     | 8                                                                                                                                                                          |
|         | CHAIN                |                                                                                                                                                      | A                                                                                                                                                                                      | <                                                                                                                                                                                      | A                                                                                                                                                                          |
|         | PDB<br>ID            |                                                                                                                                                      | 1fs2                                                                                                                                                                                   | 1652                                                                                                                                                                                   | lyrg                                                                                                                                                                       |
|         | SEQ<br>ID            |                                                                                                                                                      | 1775                                                                                                                                                                                   | 1775                                                                                                                                                                                   | 1775                                                                                                                                                                       |

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|         | PDB annotation | TA HOTTING OF A COUNTY OF A COUNTY | TWINNING, 3 MEROHEDRAL TWINNING, MEROHEDRY | ACETYLATION RNASE       | INHIBITOR,   | RIBONUCLEASE/ANGIOGEN | IN INHIBITOR | ACETYLATION, LEUCINE- | RICH REPEATS | ASPARTYL PROTEASE SIV      | PROTEINASE; HIV, AIDS, | 1101 LAIN 102, 1101 1111 12 | PROTEASE, | COMPLETA             | (PROTEASE/INHIBITOR)                     | HUMAN                 | IMMUNODEFICIENCY | VIRUS PROTEASE, ROUS | SARCOMA VIRUS 2 | PROTEASE, CRYSTAL | STRUCTURES, PROTEIN- | MEDIATED INTERACTION, 3 | VIRAL MATURATION, | COMPLEX | (PROTEASE/INHIBITOR) | HEADER | HYDROLASE HYDROLASE,         | AIDS, POLYPROTEIN, | ASFARITL FROIEASE, ACID 2 PROTEASE, |  |
|---------|----------------|------------------------------------|--------------------------------------------|-------------------------|--------------|-----------------------|--------------|-----------------------|--------------|----------------------------|------------------------|-----------------------------|-----------|----------------------|------------------------------------------|-----------------------|------------------|----------------------|-----------------|-------------------|----------------------|-------------------------|-------------------|---------|----------------------|--------|------------------------------|--------------------|-------------------------------------|--|
|         | Compound       |                                    |                                            | RIBONUCLEASE INHIBITOR; | CHAIN: NULL: |                       |              |                       |              | SIV PROTEASE; CHAIN: NULL; |                        |                             |           | STIGHT ANOCHER STICE | ROUS SARCOMA VIRUS DPOTFASE: CHAIN: A B: | INCLUSED, CITATION C. |                  |                      |                 |                   |                      |                         |                   |         |                      |        | HIV-1 PROTEASE; CHAIN: A, B; |                    |                                     |  |
| Table 5 | SEQ<br>FOLD    | score                              |                                            |                         |              |                       |              |                       |              |                            |                        |                             |           |                      | 00.31                                    |                       |                  |                      |                 |                   |                      |                         |                   |         |                      |        |                              |                    |                                     |  |
| Tak     | PMF<br>score   |                                    |                                            | 1.00                    |              |                       |              |                       |              | 0.77                       |                        |                             |           |                      |                                          |                       |                  |                      |                 |                   |                      |                         |                   |         |                      |        | 0.48                         |                    |                                     |  |
|         | Verify score   |                                    |                                            | -0.01                   |              |                       |              |                       |              | 0.30                       |                        |                             |           |                      |                                          |                       |                  |                      |                 |                   |                      |                         |                   |         |                      |        | 0.28                         | <u> </u>           | <del></del> -                       |  |
|         | Psi<br>Blast   |                                    |                                            | 1e-24                   |              |                       |              |                       |              | 3.4e-23                    |                        |                             |           |                      | 4.8e-18                                  |                       |                  |                      |                 |                   |                      |                         |                   |         |                      |        | 3.4e-39                      |                    |                                     |  |
|         | END            |                                    |                                            | 195                     | 2            |                       |              |                       |              | 348                        | )                      |                             |           |                      | 347                                      |                       |                  |                      |                 | •                 |                      |                         |                   |         |                      |        | 348                          | 2                  |                                     |  |
|         | START          |                                    |                                            | ~                       | )            |                       |              |                       |              | 248                        | 2                      |                             |           |                      | 233                                      |                       |                  |                      |                 |                   |                      |                         |                   |         |                      |        | 244                          | -                  |                                     |  |
|         | CHAIN          | )                                  |                                            |                         |              |                       |              |                       |              |                            |                        | -                           |           |                      | A                                        |                       |                  |                      |                 |                   |                      |                         |                   |         |                      |        | V                            | 4                  |                                     |  |
|         | PDB            |                                    |                                            | Jhnh                    | 701111       |                       |              |                       |              | 1275                       | Tabo                   |                             |           |                      | 1bai                                     |                       |                  |                      |                 |                   |                      |                         |                   |         |                      |        | 1150                         | i<br>i<br>i        |                                     |  |
|         | SEQ            | ÿ                                  |                                            | 1775                    | 2/1          |                       |              |                       |              | 1777                       | ///                    |                             |           |                      | 1777                                     |                       |                  |                      |                 |                   |                      |                         |                   |         |                      |        | 1777                         | · · ·              |                                     |  |

|         | PDB annotation |          | HYDROXYETHYLENE ISOSTERE INHIBITOR, SUBSTRATE 3 ANALOGUE | INHIBITOR | HYDROLASE HIV-1<br>PROTEASE, HYDROLASE | HYDROLASE HIV-1<br>PROTEASE, MUTANT,              | DIMER, INHIBITOR,           | OCCUPANCY | HYDROLASE DUTPASE,<br>DUTP PYROPHOSPHATASE; | HYDROLASE, DUTPASE,  | EIAV, TRIMERIC ENZYME, | ASPARTYL PROTEASE | HYDROLASE DUTPASE, | DUTP PYROPHOSPHATASE; | HYDROLASE, DUTPASE,  | EIAV, TRIMERIC ENZYME, | ASPARTYL PROTEASE | HYDROLASE DUTPASE; | JELLY ROLL, MERCURY | DERIVATIVE           | VIRIS/VIRAL PROTEIN        | EIGHT STRANDED BETA-              | BARREL | VIRUS/VIRAL PROTEIN        | EIGHT STRANDED BETA | BAKKEL PKULEIN | VIRUS/VIRAL PROTEIN        |
|---------|----------------|----------|----------------------------------------------------------|-----------|----------------------------------------|---------------------------------------------------|-----------------------------|-----------|---------------------------------------------|----------------------|------------------------|-------------------|--------------------|-----------------------|----------------------|------------------------|-------------------|--------------------|---------------------|----------------------|----------------------------|-----------------------------------|--------|----------------------------|---------------------|----------------|----------------------------|
|         | Compound       |          |                                                          |           | HIV-1 PROTEASE; CHAIN: A, B;           | PEPTIDE INHIBITOR; CHAIN: A,<br>B: HIV-1 PROTFASE | (RETROPEPSIN); CHAIN: C, D; |           | DEOXYURIDINE 5'-<br>TRIPHOSPHATE            | NUCLEODITOHYDROLASE; | CHAIN: NULL;           |                   | DEOXYURIDINE 5'-   | TRIPHOSPHATE          | NUCLEODITOHYDROLASE; | CHAIN: NULL;           |                   | DEOXYURIDINE 5'-   | TRIPHOSPHATE        | NUCLEOTIDOHYDROLASE; | DOI DOI VOROTEIN: CHAIN: A | I OLI OLI INOI LIIV, CILIMINI IV. | ú      | POL POLYPROTEIN; CHAIN: A; |                     |                | POL POLYPROTEIN; CHAIN: A; |
| Table 5 | SEQ            | FOLD     |                                                          |           |                                        |                                                   |                             |           |                                             |                      |                        |                   |                    |                       |                      |                        |                   |                    |                     |                      |                            |                                   |        |                            |                     |                |                            |
| Tal     | PMF            | score    |                                                          |           | 0.57                                   | 9.02                                              |                             |           | 1.00                                        |                      |                        |                   | 1.00               |                       |                      |                        |                   | 89.0               |                     |                      | 1                          | 1.00                              |        | 1.00                       |                     |                | 1.00                       |
|         | Verify         | score    |                                                          |           | 0.30                                   | 0.11                                              |                             |           | 0.32                                        |                      |                        |                   | 0.54               |                       |                      |                        |                   | 0.51               |                     |                      | 0.25                       | رد ا                              |        | -0.01                      |                     |                | 0.13                       |
|         | Psi            | Blast    |                                                          |           | 3.4e-40                                | 1.7e-38                                           |                             |           | 3.4e-23                                     |                      |                        |                   | 1.2e-26            |                       |                      |                        |                   | 1.7e-16            |                     |                      | 26.09                      | 0.06-23                           |        | 8.5e-24                    |                     |                | 6e-28                      |
|         | END            | AA       |                                                          |           | 348                                    | 348                                               |                             |           | 228                                         |                      |                        |                   | 218                |                       |                      |                        |                   | 228                |                     |                      | 200                        | 077                               |        | 242                        |                     |                | 234                        |
|         | START          | AA       |                                                          |           | 244                                    | 244                                               |                             |           | 119                                         |                      | -                      |                   | 120                |                       |                      |                        |                   | 124                |                     |                      | 110                        | 119                               |        | 119                        |                     |                | 122                        |
|         | CHAIN          | А        |                                                          |           | A                                      | C                                                 |                             |           |                                             |                      |                        |                   |                    |                       |                      |                        |                   | A                  |                     |                      |                            | <b>4</b>                          |        | A                          |                     |                | A                          |
|         | PDB            | <u>A</u> |                                                          | -         | 1bwb                                   | 1daz                                              |                             | •••       | 1dun                                        |                      |                        |                   | 1dun               |                       |                      |                        |                   | leuw               |                     |                      | ,<br>E                     | JI/d                              |        | 1 <i>f7</i> r              | !                   |                | 1f7r                       |
|         | SEQ            | ВŞ       |                                                          |           | 1777                                   | 1777                                              | 2                           |           | 1777                                        |                      |                        |                   | 1777               |                       |                      |                        |                   | 1777               |                     |                      | 1                          | 1///                              |        | 1777                       |                     |                | 1777                       |

|         | PDB annotation |         | EIGHT STRANDED BETA<br>BARREL PROTEIN | HYDROLASE (ACID             | (ACID PROTEINASE), RNA- | DIRECTED DNA | POLYMERASE, 2 ASPARTYL | PROTEASE, | ENDONUCLEASE,<br>POLYPROTEIN | HYDROLASE HYDROLASE       |                          |                          |                             |                  |                        |        |                          |                          |                             |                  |                        |        |                |                   |                        |                              |                      |                     |                                          |  |
|---------|----------------|---------|---------------------------------------|-----------------------------|-------------------------|--------------|------------------------|-----------|------------------------------|---------------------------|--------------------------|--------------------------|-----------------------------|------------------|------------------------|--------|--------------------------|--------------------------|-----------------------------|------------------|------------------------|--------|----------------|-------------------|------------------------|------------------------------|----------------------|---------------------|------------------------------------------|--|
|         | Compound       |         |                                       | EIAV PROTEASE; CHAIN: NULL; |                         |              |                        |           |                              | HIV-1 PROTEASE; CHAIN: A; | HYDROLASE(ACID PROTEASE) | HIV-1 PROTEASE (TETHERED | DIMER LINKED BY 1HVC 3 GLY- | GLY-SER-SER-GLY) | COMPLEXED WITH A-76928 | 1HVC 4 | HYDROLASE(ACID PROTEASE) | HIV-1 PROTEASE (TETHERED | DIMER LINKED BY 1HVC 3 GLY- | GLY-SER-SER-GLY) | COMPLEXED WITH A-76928 | 1HVC 4 | HYDROLASE(ACID | PROTEINASE) HUMAN | IMMUNODEFICIENCY VIRUS | TYPE 2 (HIV-2) PROTEASE 1IDA | 3 COMPLEXED WITH THE | INHIBITOR BILA 1906 | CONTAINING THE 1IDA 4 HYDROXYETHYI.AMINE |  |
| Table 5 | SEQ            | score   |                                       | 58.04                       |                         |              |                        |           |                              |                           | 57.17                    |                          |                             |                  |                        |        |                          |                          |                             |                  |                        |        |                |                   |                        | ,                            |                      |                     |                                          |  |
| Ta      | PMF            | score   |                                       |                             |                         |              |                        |           |                              | 0.35                      |                          |                          |                             |                  |                        |        | 0.37                     |                          |                             |                  | _                      |        | 0.64           |                   |                        |                              |                      |                     |                                          |  |
|         | Verify         | score   |                                       |                             |                         |              |                        |           |                              | 0.36                      |                          |                          |                             |                  |                        |        | 0.16                     |                          |                             |                  |                        |        | 0.22           |                   |                        |                              |                      |                     |                                          |  |
|         | Psi            | Blast   |                                       | 1.2e-14                     |                         |              |                        |           |                              | 1.7e-42                   | 6.8e-43                  |                          |                             |                  |                        |        | 6.8e-43                  |                          |                             |                  |                        |        | 6.8e-26        |                   |                        |                              |                      |                     |                                          |  |
|         | END            | AA<br>_ |                                       | 348                         |                         |              |                        |           |                              | 348                       | 348                      |                          |                             |                  |                        |        | 348                      |                          |                             |                  |                        |        | 347            | _                 |                        |                              |                      |                     |                                          |  |
|         | START          | AA      |                                       | 244                         |                         |              |                        |           |                              | 179                       | 122                      |                          |                             |                  |                        |        | 177                      |                          |                             |                  |                        |        | 244            |                   |                        |                              |                      |                     |                                          |  |
|         | CHAIN          | a       |                                       |                             |                         |              |                        |           |                              | A                         |                          |                          |                             |                  |                        |        |                          |                          |                             |                  |                        |        | Ą              |                   |                        |                              |                      |                     |                                          |  |
|         | PDB            | <br>A   |                                       | 1 fmb                       |                         |              |                        |           | T-21-31                      | 1261                      | 1hvc                     |                          |                             |                  |                        |        | 1hvc                     |                          |                             |                  |                        |        | 1ida           |                   |                        |                              |                      |                     |                                          |  |
|         | SEQ            | A Ş     |                                       | 1777                        |                         |              |                        |           |                              | 1777                      | 1777                     |                          |                             |                  |                        |        | 1777                     |                          |                             |                  |                        |        | 1777           |                   |                        | ·                            |                      |                     |                                          |  |

|         | PDB annotation |          |                           | COMPLEX (ASPARTYL PROTEASE/INHIBITOR) HIV-          | 1 PR; HYDROLASE,<br>ASPARTYL PROTEINASE,<br>AIDS, PEPTIDE, INHIBITOR |                                      |                                                     |                                            | COMPLEX (TWO DNA-<br>BINDING PROTEINS/DNA)        | MAT ALPHA-2; COMPLEX       | (I WO DINA-BINDING PROTFINS/DNA) COMPLEX | 2 DNA-BINDING PROTEIN. | DNA. TRANSCRIPTION | REGULATION | COMPLEX (TWO DNA-        | BINDING PROTEINS/DNA) | MAT ALPHA-2; COMPLEX       | (TWO DNA-BINDING | PROTEINS/DNA), COMPLEX, | 2 DINA-BIINDIING FROI EIIN, | DINA, I KANSCKIF I I ON<br>PEGI II ATTON | The continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue of the continue o |                                                 |
|---------|----------------|----------|---------------------------|-----------------------------------------------------|----------------------------------------------------------------------|--------------------------------------|-----------------------------------------------------|--------------------------------------------|---------------------------------------------------|----------------------------|------------------------------------------|------------------------|--------------------|------------|--------------------------|-----------------------|----------------------------|------------------|-------------------------|-----------------------------|------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------|
|         | Compound       |          | DIPEPTIDE ISOSTERE 1IDA 5 | HIV-1 PROTEASE; A CYCLIC PHE-ILE-VAL PEPTIDOMIMETIC | INHIBITOR; CHAIN: C;                                                 | HYDROLASE(ACID<br>PROTEINASE) SIMIAN | IMMUNODEFICIENCY VIRUS (SIV) PROTEINASE 1SIP 3 (SIV | MAC251-32H ISOLATE)<br>(E.C.3.4.23) 1SIP 4 | MATING-TYPE PROTEIN A-1;<br>CHAIN: A: MATING-TYPE | PROTEIN ALPHA-2; CHAIN: B; | DNA; CHAIN: C;                           |                        |                    |            | MATING-TYPE PROTEIN A-1; | CHAIN: A; MATING-TYPE | PROTEIN ALPHA-2; CHAIN: B; | DNA; CHAIN: C;   |                         |                             |                                          | CONTRIBUTE TO THE PRINCE                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       | COMPLEA(DINA BINDING<br>PROTEIN/DNA) MAT ALPHA2 |
| Table 5 | SEQ            | FOLD     |                           |                                                     |                                                                      |                                      |                                                     |                                            |                                                   |                            |                                          |                        |                    |            |                          |                       |                            |                  |                         |                             |                                          |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |                                                 |
| Tal     | PMF            | score    |                           | 0.92                                                |                                                                      | 0:30                                 |                                                     |                                            | 0.13                                              |                            |                                          |                        |                    |            | 0.16                     |                       |                            |                  |                         |                             |                                          | 000                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            | 0.28                                            |
|         | Verify         | score    |                           | 0.25                                                |                                                                      | -0.05                                |                                                     |                                            | -0.37                                             |                            |                                          |                        |                    |            | -0.58                    |                       |                            |                  |                         |                             |                                          | 9                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | -0.49                                           |
|         | Psi            | Blast    |                           | 6.8e-38                                             |                                                                      | 3.4e-27                              |                                                     | •                                          | 1.4e-14                                           |                            |                                          |                        |                    |            | 1.1e-15                  |                       |                            |                  |                         |                             |                                          |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | 2.4e-15                                         |
|         | END            | AA       |                           | 342                                                 |                                                                      | 348                                  |                                                     |                                            | 138                                               |                            |                                          |                        |                    |            | 137                      |                       |                            |                  |                         |                             |                                          | 9                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | 129                                             |
| •       | START          |          |                           | 244                                                 |                                                                      | 244                                  | -                                                   |                                            | 70                                                |                            |                                          |                        |                    |            | 72                       |                       |                            |                  |                         |                             |                                          |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | 20                                              |
|         | CHAIN          | <u></u>  |                           | A                                                   |                                                                      |                                      |                                                     |                                            | В                                                 |                            |                                          |                        |                    |            | В                        | 1                     |                            |                  |                         |                             |                                          |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | ن<br>د                                          |
|         | PDB            | <u> </u> |                           | 1mtr                                                |                                                                      | 1sip                                 |                                                     |                                            | 1akh                                              |                            |                                          |                        |                    |            | 1akh                     |                       |                            |                  |                         |                             |                                          |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | lapl                                            |
|         | SEQ            | ВŞ       |                           | 1777                                                |                                                                      | 1777                                 |                                                     |                                            | 1788                                              |                            |                                          |                        |                    |            | 1788                     | )                     |                            |                  |                         |                             |                                          |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | 1788                                            |

|         | PDB annotation |            |                                                |                                             |                                                | PROTEIN/DNA<br>HOMEODOMAIN, DNA,                          | COMPLEX, DNA-BINDING PROTEIN, PROTEIN/DNA | TRANSCRIPTION/DNA      | ULTRABITHORAX; PBX    | HOMEODOMAIN,             | HOMEOTIC PROTEINS,          | DEVELOPMENT, 2 | SPECIFICITY | GENE REGULATION PBX1;<br>HOMEODOMAIN | COMPLEX              | (TRANSCRIPTION/HOMEOB OX/DNA) PHEROMONE                  | RECEPTOR TRANSCRIPTION       | FACTOR; MATING-TYPE        | PROTEIN ALPHA-2; | TRANSCRIPTION | KEGULATION,<br>TRANSCRIPTIONAL | REPRESSION, 2 DNA- | BINDING PROTEIN,<br>COMPLEX |
|---------|----------------|------------|------------------------------------------------|---------------------------------------------|------------------------------------------------|-----------------------------------------------------------|-------------------------------------------|------------------------|-----------------------|--------------------------|-----------------------------|----------------|-------------|--------------------------------------|----------------------|----------------------------------------------------------|------------------------------|----------------------------|------------------|---------------|--------------------------------|--------------------|-----------------------------|
|         | Compound       |            | HOMEODOMAIN COMPLEXED WITH OPERATOR DNA 1APL 3 | COMPLEX(DNA BINDING PROTEIN/DNA) MAT ALPHA2 | HOMEODOMAIN COMPLEXED WITH OPERATOR DNA 1APL 3 | HOMEOBOX PROTEIN HOX-B1;<br>CHAIN: A: PBX1: CHAIN: B: DNA | CHAIN: D; DNA CHAIN: E;                   | ULTRABITHORAX HOMEOTIC | PROTEIN IV; CHAIN: A; | EXTRADENTICLE: CHAIN: B; | DNA (5'- CHAIN: C; DNA (5'- | CHAIN: D;      |             | HOMEOBOX PROTEIN PBX1;<br>CHAIN: A;  | MCM1 TRANSCRIPTIONAL | REGULATOR; CHAIN: A, B; MAT<br>AI, PHA-2 TRANSCRIPTIONAL | REPRESSOR; CHAIN: C, D; STE6 | OPERATOR DNA; CHAIN: E, F; |                  |               |                                |                    |                             |
| Table 5 | SEQ            | FOLD score |                                                |                                             |                                                |                                                           |                                           |                        |                       |                          |                             |                |             |                                      |                      |                                                          |                              |                            |                  |               |                                |                    |                             |
| Tak     | PMF            | score      |                                                | 0.18                                        |                                                | 0.46                                                      |                                           | 0.92                   |                       |                          |                             |                |             | 0.88                                 | 0.10                 |                                                          |                              |                            |                  |               |                                |                    |                             |
|         | Verify         | score      |                                                | -0.05                                       |                                                | -0.20                                                     |                                           | 0.12                   |                       |                          |                             |                |             | 0.19                                 | -0.16                |                                                          |                              |                            |                  |               |                                |                    |                             |
|         | Psi            | Blast      |                                                | 8.5e-14                                     |                                                | 1.4e-20                                                   | •                                         | 6.8e-19                |                       |                          |                             |                |             | 1.5e-17                              | 6.8e-15              |                                                          |                              |                            |                  |               |                                |                    |                             |
|         | END            | AA         |                                                | 129                                         |                                                | 134                                                       |                                           | 131                    |                       |                          |                             |                |             | 131                                  | 129                  |                                                          |                              |                            |                  |               |                                |                    |                             |
|         | START          | AA         |                                                | 73                                          |                                                | 72                                                        |                                           | 74                     |                       | -                        |                             |                |             | 75                                   | 54                   |                                                          |                              |                            |                  |               |                                |                    |                             |
|         | CHAIN          | А          |                                                | S                                           |                                                | В                                                         |                                           | 2                      | 1                     |                          |                             |                |             | A                                    | C                    |                                                          |                              |                            |                  |               |                                |                    |                             |
|         | PDB            | <u> </u>   |                                                | lapl                                        |                                                | 1672                                                      |                                           | 1581                   |                       | ,                        | _=~-                        |                |             | 1du6                                 | 1mnm                 |                                                          |                              |                            |                  |               |                                |                    |                             |
|         | SEQ            | A È        |                                                | 1788                                        |                                                | 1788                                                      |                                           | 1788                   | 2                     |                          |                             |                |             | 1788                                 | 1788                 |                                                          |                              |                            |                  |               |                                |                    |                             |

|         | PDB annotation | (TRANSCRIPTION/HOMEOB<br>OX/DNA) | RNA-BINDING<br>PROTEIN/RNA TRA PRE- | MRNA; SPLICING<br>REGULATION, RNP<br>DOMAIN, RNA COMPLEX       | RNA-BINDING<br>PROTEIN/RNA TRA PRE-          | MRNA; SPLICING | REGULATION, RNP<br>DOMAIN, RNA COMPLEX | RNA-BINDING                  | PROTEIN/RNA TRA PRE- | MRNA; SPLICING                        | REGULATION, RNP                                                                 | DOMAIN, RNA COMPLEX | RNA-BINDING     | PROTEIN/RNA TRA PRE- | MRNA; SPLICING | REGULATION, RNP             | DOMAIN, KNA COMPLEX | GENE REGULATION/RNA<br>POLY(A) BINDING PROTEIN            | 1, PABP 1; RRM, PROTEIN- | RNA COMPLEX, GENE | REGULATION/RNA |   | GENE REGULATION/RNA<br>POLY(A) BINDING PROTEIN |
|---------|----------------|----------------------------------|-------------------------------------|----------------------------------------------------------------|----------------------------------------------|----------------|----------------------------------------|------------------------------|----------------------|---------------------------------------|---------------------------------------------------------------------------------|---------------------|-----------------|----------------------|----------------|-----------------------------|---------------------|-----------------------------------------------------------|--------------------------|-------------------|----------------|---|------------------------------------------------|
|         | Compound       |                                  |                                     | R(P*GP*UP*UP*GP*UP*UP*UP*<br>UP*UP*UP*U)- CHAIN: P, Q; Ri<br>D | SXL-LETHAL PROTEIN; CHAIN: R. A. R. RNA (5'- | P*GP*UP*UP*    | UP*UP*UP*UP*U. CHAIN: P, Q; R          | SXL-LETHAL PROTEIN; CHAIN: R |                      | $	ext{R(P*GP*UP*UP*UP*} \mid 	ext{N}$ | $\mathrm{UP}*\mathrm{UP}*\mathrm{UP}*\mathrm{UP}*\mathrm{U}$ - CHAIN: P, Q;   R | Q                   | PROTEIN; CHAIN: |                      |                | UP*UP*UP*U-CHAIN: P, Q;   R |                     | POLYDENYLATE BINDING PROTEIN 1: CHAIN: A. B. C. D. E.   P |                          | P*AP*AP*A         |                |   | LATE BINDING<br>CHAIN: A, B, C, D, E,          |
| Table 5 | SEQ<br>FOLD    |                                  | 96.30                               |                                                                | 01                                           |                |                                        |                              |                      | <u> </u>                              |                                                                                 |                     |                 | <u> </u>             |                |                             |                     |                                                           |                          |                   |                |   |                                                |
| Tab     | PMF<br>score   |                                  |                                     | , , , , , ,                                                    | 1.00                                         |                | ,                                      | 1.00                         |                      |                                       |                                                                                 |                     | 0.29            |                      |                |                             |                     | 1.00                                                      |                          |                   |                |   | 1.00                                           |
|         | Verify         |                                  |                                     |                                                                | 68.0                                         |                |                                        | 0.81                         |                      |                                       |                                                                                 |                     | -0.20           |                      |                |                             |                     | 0.87                                                      |                          |                   |                |   | 1.04                                           |
|         | Psi<br>Blast   |                                  | 8e-44                               |                                                                | 8e-44                                        |                |                                        | 4e-43                        |                      | -                                     |                                                                                 |                     | 1.7e-30         |                      |                |                             |                     | 1.6e-45                                                   |                          |                   |                |   | 1.4e-27                                        |
|         | END<br>AA      |                                  | 323                                 |                                                                | 323                                          |                |                                        | 425                          |                      |                                       |                                                                                 |                     | 131             |                      |                |                             |                     | 329                                                       |                          |                   |                |   | 329                                            |
|         | START<br>AA    |                                  | 154                                 |                                                                | 157                                          |                |                                        | 248                          |                      |                                       |                                                                                 |                     | 3               |                      |                |                             |                     | 157                                                       |                          |                   |                |   | 158                                            |
|         | CHAIN          |                                  | A                                   |                                                                | A                                            |                |                                        | A                            |                      |                                       |                                                                                 |                     | A               |                      |                |                             |                     | A                                                         |                          |                   |                |   | A                                              |
|         | PDB<br>ID      |                                  | 1b7f                                |                                                                | 1b7f                                         |                |                                        | 1h7f                         |                      |                                       |                                                                                 |                     | 1b7f            |                      |                |                             |                     | 1cvj                                                      |                          | -                 |                | _ | 1cvj                                           |
|         | SEQ<br>EQ      | ġ.                               | 1792                                |                                                                | 1792                                         |                |                                        | 1792                         |                      |                                       |                                                                                 |                     | 1792            |                      |                |                             |                     | 1792                                                      |                          |                   |                |   | 1792                                           |

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|         | PDB annotation |          | I, PABP I; RRM, PROTEIN-<br>RNA COMPLEX, GENE<br>REGULATION/RNA                                  | GENE REGULATION/RNA POLY(A) BINDING PROTEIN 1, PABP 1; RRM, PROTEIN- RNA COMPLEX, GENE REGULATION/RNA                                         | GENE REGULATION/RNA POLY(A) BINDING PROTEIN 1, PABP 1; RRM, PROTEIN- RNA COMPLEX, GENE REGULATION/RNA                                  | GENE REGULATION/RNA POLY(A) BINDING PROTEIN 1, PABP 1; RRM, PROTEIN- RNA COMPLEX, GENE REGULATION/RNA                                     | GENE REGULATION/RNA<br>POLY(A) BINDING PROTEIN<br>1, PABP 1; RRM, PROTEIN-<br>RNA COMPLEX, GENE<br>REGULATION/RNA                                         | GENE REGULATION/RNA<br>POLY(A) BINDING PROTEIN<br>1, PABP 1; RRM, PROTEIN-    |
|---------|----------------|----------|--------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------|
|         | Compound       |          | F, G, H; RNA (5'-<br>R(*AP*AP*AP*AP*AP*AP*A<br>P*AP*AP*A)-3'); CHAIN: M, N, O,<br>P, Q, R, S, T; | POLYDENYLATE BINDING PROTEIN 1; CHAIN: A, B, C, D, E, F, G, H; RNA (5'- R(*AP*AP*AP*AP*AP*AP*A P*AP*AP*A)-3'); CHAIN: M, N, O, P, Q, R, S, T; | POLYDENYLATE BINDING PROTEIN 1; CHAIN: A, B, C, D, E, F, G, H; RNA (5'- R(*AP*AP*AP*AP*AP*A P*AP*AP*A); CHAIN: M, N, O, P, Q, R, S, T; | POLYDENYLATE BINDING PROTEIN 1; CHAIN: A, B, C, D, E, F, G, H; RNA (5'- R(*AP*AP*AP*AP*AP*AP*A P*AP*AP*A); CHAIN: M, N, O, P, Q, R, S, T; | POLYDENYLATE BINDING<br>PROTEIN 1; CHAIN: A, B, C, D, E,<br>F, G, H; RNA (5'-<br>R(*AP*AP*AP*AP*AP*AP*A<br>P*AP*AP*A):; CHAIN: M, N, O,<br>P, Q, R, S, T; | POLYDENYLATE BINDING<br>PROTEIN 1; CHAIN: A, B, C, D, E,<br>F, G, H; RNA (5'- |
| Table 5 | SEQ            | FOLD     |                                                                                                  |                                                                                                                                               |                                                                                                                                        | 223.38                                                                                                                                    |                                                                                                                                                           |                                                                               |
| Tal     | PMF            | score    |                                                                                                  | 1.00                                                                                                                                          | 1.00                                                                                                                                   |                                                                                                                                           | 1.00                                                                                                                                                      | 1.00                                                                          |
|         | Verify         | score    |                                                                                                  | 1.01                                                                                                                                          | 0.97                                                                                                                                   |                                                                                                                                           | 0.81                                                                                                                                                      | 1.06                                                                          |
|         | Psi            | Blast    |                                                                                                  | 4e-43                                                                                                                                         | 1.2e-28                                                                                                                                | 8.5e-55                                                                                                                                   | 8.5e-55                                                                                                                                                   | 1.6e-37                                                                       |
|         | END            | AA       |                                                                                                  | 426                                                                                                                                           | 422                                                                                                                                    | 236                                                                                                                                       | 236                                                                                                                                                       | 313                                                                           |
|         | START          | AA       |                                                                                                  | 249                                                                                                                                           | 250                                                                                                                                    | 89                                                                                                                                        | 69                                                                                                                                                        | 157                                                                           |
|         | CHAIN          | <u> </u> |                                                                                                  | ₩                                                                                                                                             | A                                                                                                                                      | A                                                                                                                                         | ¥.                                                                                                                                                        | В                                                                             |
|         | PDB            | <u> </u> |                                                                                                  | 1cvj                                                                                                                                          | 1cvj                                                                                                                                   | 1cvj                                                                                                                                      | lcvj                                                                                                                                                      | 1cvj                                                                          |
|         | SEQ            | e è      | ġ.                                                                                               | 1792                                                                                                                                          | 1792                                                                                                                                   | 1792                                                                                                                                      | 1792                                                                                                                                                      | 1792                                                                          |

|         | PDB annotation |            | RNA COMPLEX, GENE<br>REGULATION/RNA                                            | GENE REGULATIONRNA<br>POLY(A) BINDING PROTEIN<br>1, PABP 1; RRM, PROTEIN-     | RNA COMPLEX, GENE<br>REGULATION/RNA                                               | GENE REGULATION/RNA<br>POLY(A) BINDING PROTEIN           | I, FABE 1, MAN, TRO LEINE<br>RNA COMPLEX, GENE<br>PEGITI ATTONIRNA            |                                                    | GENE REGULATION/RNA  | POLY(A) BINDING PROTEIN<br>1 PABP 1: RRM. PROTEIN- | RNA COMPLEX, GENE                            | REGULATION/RNA                                 | GENE REGULATION/RNA  | POLY(A) BINDING FROTEIN<br>1, PABP 1; RRM, PROTEIN-   | RNA COMPLEX, GENE         | REGULATION/RNA                                    | GENE REGULATION/RNA  | POLY(A) BINDING PROTEIN          | I, FABE 1, KKW, FRO LEIN-<br>RNA COMPLEX, GENE |
|---------|----------------|------------|--------------------------------------------------------------------------------|-------------------------------------------------------------------------------|-----------------------------------------------------------------------------------|----------------------------------------------------------|-------------------------------------------------------------------------------|----------------------------------------------------|----------------------|----------------------------------------------------|----------------------------------------------|------------------------------------------------|----------------------|-------------------------------------------------------|---------------------------|---------------------------------------------------|----------------------|----------------------------------|------------------------------------------------|
|         | Compound       |            | R(*AP*AP*AP*AP*AP*AP*AP*A<br>P*AP*AP*A)-3'); CHAIN: M, N, O,<br>P, Q, R, S, T; | POLYDENYLATE BINDING<br>PROTEIN 1; CHAIN: A, B, C, D, E,<br>F, G, H; RNA (5'- | R(*AP*AP*AP*AP*AP*AP*AP*AP*A<br>P*AP*AP*A)-3'); CHAIN: M, N, O,<br>P, Q, R, S, T; | POLYDENYLATE BINDING<br>PROTEIN 1; CHAIN: A, B, C, D, E, | F, G, H; KNA (2-<br>R(*AP*AP*AP*AP*AP*AP*A<br>B**D**AP*A) 211. CHANI, M. N. O | P. AF. AF. A. J.; CHAIN: IM, IN, O, P, Q, R, S, T; | POLYDENYLATE BINDING | PROTEIN 1; CHAIN: A, B, C, D, E,                   | I, C, M, | P*AP*AP*A)-3'); CHAIN: M, N, O, P, O, R, S, T; | POLYDENYLATE BINDING | PROTEIN 1; CHAIN: A, B, C, D, E,<br>F. G. H: RNA (5'- | R(*AP*AP*AP*AP*AP*AP*AP*A | P*AP*AP*A)-3'); CHAIN: M, N, O,<br>P, O, R, S, T; | POLYDENYLATE BINDING | PROTEIN 1; CHAIN: A, B, C, D, E, | F, G, H; KNA (2"-<br>R(*AP*AP*AP*AP*AP*AP*A    |
| Table 5 | SEQ            | FOLD score |                                                                                |                                                                               |                                                                                   |                                                          |                                                                               |                                                    |                      |                                                    |                                              |                                                | 188.53               |                                                       |                           |                                                   |                      |                                  |                                                |
| Tab     | PMF            | score      |                                                                                | 1.00                                                                          |                                                                                   | 1.00                                                     |                                                                               |                                                    | 90.0                 |                                                    |                                              |                                                |                      |                                                       |                           |                                                   | 1.00                 |                                  |                                                |
|         | Verify         | score      |                                                                                | 0.83                                                                          |                                                                                   | 0.93                                                     |                                                                               |                                                    | -0.03                |                                                    |                                              |                                                |                      |                                                       |                           |                                                   | 0.89                 |                                  |                                                |
|         | Psi            | Blast      |                                                                                | 6.8e-23                                                                       |                                                                                   | 6e-38                                                    |                                                                               |                                                    | 6.8e-29              |                                                    |                                              |                                                | 3.4e-46              |                                                       |                           |                                                   | 3.4e-46              |                                  |                                                |
|         | END            | AA         |                                                                                | 309                                                                           |                                                                                   | 417                                                      |                                                                               |                                                    | 130                  |                                                    |                                              |                                                | 222                  |                                                       |                           |                                                   | 216                  |                                  |                                                |
|         | START          | AA         |                                                                                | 158                                                                           |                                                                                   | 249                                                      |                                                                               |                                                    | 3                    |                                                    |                                              | _                                              | 89                   |                                                       |                           |                                                   | 69                   |                                  |                                                |
|         | CHAIN          | А          |                                                                                | В                                                                             |                                                                                   | В                                                        |                                                                               |                                                    | В                    |                                                    |                                              |                                                | В                    |                                                       |                           |                                                   | В                    |                                  |                                                |
|         | PDB            | А          |                                                                                | 1cvj                                                                          |                                                                                   | 1cvj                                                     |                                                                               |                                                    | lcvj                 | 3                                                  |                                              |                                                | 1cvj                 |                                                       |                           |                                                   | 1cvi                 | ·<br>                            |                                                |
|         | SEQ            | í A Ş      |                                                                                | 1792                                                                          |                                                                                   | 1792                                                     |                                                                               |                                                    | 1792                 |                                                    |                                              |                                                | 1792                 |                                                       |                           |                                                   | 1792                 |                                  | <del></del>                                    |

|         | ation          |               | IA                                             | ON/RNA               | G PROTEIN                        | ROTEIN.                  | GENE                   | ١A                              |                | ION/RNA              | G PROTEIN                        | ROTEIN-                  | GENE                   | NA<br>VA                        |                | ION/RNA              | G PROTEIN                        | PROTEIN-                 | GENE                   | VA.                             |                | ION/RNA              | G PROTEIN                        | PROTEIN-                 | GENE                      | NA                              |                |                            | ESTED                  | OKNOT RNA             | POTEIN                     | NOTEIN                 |
|---------|----------------|---------------|------------------------------------------------|----------------------|----------------------------------|--------------------------|------------------------|---------------------------------|----------------|----------------------|----------------------------------|--------------------------|------------------------|---------------------------------|----------------|----------------------|----------------------------------|--------------------------|------------------------|---------------------------------|----------------|----------------------|----------------------------------|--------------------------|---------------------------|---------------------------------|----------------|----------------------------|------------------------|-----------------------|----------------------------|------------------------|
|         | PDB annotation |               | REGULATION/RNA                                 | GENE REGULATION/RNA  | POLY(A) BINDING PROTEIN          | 1, PABP 1; RRM, PROTEIN- | RNA COMPLEX, GENE      | REGULATION/RNA                  |                | GENE REGULATION/RNA  | POLY(A) BINDING PROTEIN          | 1, PABP 1; RRM, PROTEIN- | RNA COMPLEX, GENE      | REGULATION/RNA                  |                | GENE REGULATION/RNA  | POLY(A) BINDING PROTEIN          | 1, PABP 1; RRM, PROTEIN- | RNA COMPLEX, GENE      | REGULATION/RNA                  |                | GENE REGULATION/RNA  | POLY(A) BINDING PROTEIN          | 1, PABP 1; RRM, PROTEIN- | RNA COMPLEX, GENE         | REGULATION/RNA                  |                | RNA BINDING                | PROTEIN/RNA NESTED     | DOUBLE PSEUDOKNOT RNA | BNA BRITING BROTEIN        | KINA BIINDIING F       |
|         | Compound       |               | P*AP*AP*A)-3'); CHAIN: M, N, O, P, Q, R, S, T; | POLYDENYLATE BINDING | PROTEIN 1; CHAIN: A, B, C, D, E, | F, G, H; RNA (5'-        | R(*AP*AP*AP*AP*AP*AP*A | P*AP*AP*A)-3'); CHAIN: M, N, O, | P, Q, R, S, T; | POLYDENYLATE BINDING | PROTEIN 1; CHAIN: A, B, C, D, E, | F, G, H; RNA (5'-        | R(*AP*AP*AP*AP*AP*AP*A | P*AP*AP*A)-3'); CHAIN: M, N, O, | P, Q, R, S, T; | POLYDENYLATE BINDING | PROTEIN 1; CHAIN: A, B, C, D, E, | F, G, H; RNA (5'-        | R(*AP*AP*AP*AP*AP*AP*A | P*AP*AP*A)-3'); CHAIN: M, N, O, | P, Q, R, S, T; | POLYDENYLATE BINDING | PROTEIN 1; CHAIN: A, B, C, D, E, | F, G, H; RNA (5'-        | R(*AP*AP*AP*AP*AP*AP*AP*A | P*AP*AP*A)-3'); CHAIN: M, N, O, | P, Q, R, S, T; | U1A PROTEIN; CHAIN: A; HDV | RIBOZYME SELF-CLEAVED; | CHAIN: B;             | THI ANTHOENI C. CHIAIN. A. | HO ANTIGENC; CHAIN: A; |
| Table 5 | SEQ            | FOLD<br>score |                                                |                      |                                  |                          |                        |                                 |                |                      |                                  |                          |                        |                                 |                |                      |                                  |                          |                        |                                 |                |                      |                                  |                          |                           |                                 |                |                            |                        |                       |                            |                        |
| Tal     | PMF            | score         |                                                | 1.00                 |                                  |                          |                        |                                 |                | 1.00                 |                                  |                          |                        |                                 |                | 1.00                 |                                  |                          |                        |                                 |                | 1.00                 |                                  |                          |                           |                                 |                | 1.00                       |                        |                       | 5                          | 1.08                   |
|         | Verify         | score         |                                                | 98.0                 |                                  |                          |                        |                                 |                | 0.56                 |                                  | _                        |                        |                                 |                | 69.0                 |                                  |                          |                        |                                 |                | 98.0                 |                                  |                          |                           |                                 |                | 0.87                       |                        |                       |                            | 0.85                   |
|         | Psi            | Blast         |                                                | 8e-30                |                                  |                          |                        |                                 |                | 4e-28                |                                  |                          |                        |                                 |                | 6e-31                |                                  |                          |                        |                                 |                | 2e-28                |                                  |                          |                           |                                 |                | 6e-21                      |                        |                       |                            | 7e-71                  |
|         | END            | AA            |                                                | 301                  |                                  |                          |                        |                                 |                | 403                  |                                  |                          |                        |                                 |                | 302                  |                                  |                          |                        |                                 |                | 403                  |                                  |                          |                           |                                 |                | 427                        |                        |                       | 10.                        | 427                    |
|         | START          | AA            |                                                | 157                  |                                  |                          |                        |                                 |                | 249                  |                                  |                          |                        |                                 |                | 157                  |                                  |                          |                        |                                 |                | 249                  |                                  |                          |                           |                                 |                | 352                        |                        |                       | 9                          | 352                    |
|         | CHAIN          |               |                                                | L                    |                                  |                          |                        |                                 |                | נדי                  |                                  |                          |                        |                                 |                | H                    | 1                                |                          |                        |                                 |                | Н                    |                                  |                          |                           |                                 |                | A                          |                        |                       |                            | А                      |
|         | PDB            |               |                                                | 1cvi                 | ,                                |                          | -                      |                                 |                | 1cvj                 | ,                                |                          |                        |                                 |                | 1cvi                 |                                  |                          | _                      |                                 |                | Icvj                 | 1                                |                          |                           |                                 |                | 1cx0                       |                        |                       |                            | 1d8z                   |
|         | SEQ            | <u> </u>      |                                                | 1792                 |                                  |                          |                        |                                 |                | 1792                 |                                  |                          |                        |                                 |                | 1792                 | 1                                |                          |                        |                                 |                | 1792                 |                                  |                          |                           |                                 |                | 1797                       | 1                      |                       |                            | 1792                   |

|         | PDB annotation  |       | RNA-BINDING DOMAIN | RNA BINDING PROTEIN<br>RNA-BINDING DOMAIN | RNA BINDING PROTEIN<br>RNA-BINDING DOMAIN | RIBONUCLEOPROTEIN | U1A117;              | RIBONUCLEOPROTEIN, RNP | DOMAIN, SPLICEOSOME | KIBOINOCLEOFRO LELIN | PIBONIICI EOPROTEIN RNP | DOMAIN. SPLICEOSOME | STRUCTURAL PROTEIN         | PROTEIN C23; RNP, RBD, | RRM, RNA BINDING | DOMAIN, NUCLEOLUS | STRUCTURAL PROTEIN        | PROTEIN C23; RNP, RBD, | RRM, RNA BINDING | DOMAIN, NUCLEOLUS | NUCLEAR PROTEIN        | HETEROGENEOUS | NUCLEAR | RIBONUCLEOPROTEIN A1, | NUCLEAR PROTEIN, HNRNP, | RBD, RRM, RNP, RNA | BINDING, 2 | RIBONUCLEOPROTEIN | NUCLEAR PROTEIN<br>HETEROGENEOUS |
|---------|-----------------|-------|--------------------|-------------------------------------------|-------------------------------------------|-------------------|----------------------|------------------------|---------------------|----------------------|-------------------------|---------------------|----------------------------|------------------------|------------------|-------------------|---------------------------|------------------------|------------------|-------------------|------------------------|---------------|---------|-----------------------|-------------------------|--------------------|------------|-------------------|----------------------------------|
|         | Compound        |       |                    | HU ANTIGEN C; CHAIN: A;                   | HU ANTIGEN C; CHAIN: A;                   | U1 SMALL NUCLEAR  | RIBONUCLEOPROTEIN A; | CHAIN: NULL;           |                     | UI SMALL NUCLEAR     | KIBUNUCLEOFROIEIN A,    | CHAIN: NOLL;        | NITCLEOLIN RBD1: CHAIN: A: |                        |                  |                   | NUCLEOLIN RBD1; CHAIN: A; |                        |                  |                   | HNRNP A1; CHAIN: NULL; |               |         |                       |                         |                    |            |                   | HNRNP A1; CHAIN: NULL;           |
| Table 5 | SEQ<br>FOLD     | score |                    |                                           |                                           |                   |                      |                        |                     | _                    |                         |                     |                            |                        |                  |                   |                           |                        |                  |                   | 87.90                  |               |         |                       |                         |                    |            |                   |                                  |
| Tab     | PMF<br>score    |       |                    | 0.87                                      | 1.00                                      | 1.00              |                      |                        |                     | 0.47                 |                         |                     | 0.31                       | 1                      |                  |                   | -0.02                     | !                      |                  |                   |                        |               |         |                       |                         |                    |            |                   | 1.00                             |
|         | Verify<br>score | -     |                    | 0.20                                      | 1.04                                      | 0.74              |                      |                        |                     | 0.55                 |                         |                     | 0.53                       |                        |                  |                   | 0.23                      |                        |                  |                   |                        |               |         |                       |                         |                    |            |                   | 0.91                             |
|         | Psi<br>Blast    |       |                    | 8.5e-23                                   | 1e-20                                     | 4e-20             |                      |                        |                     | 1.4e-11              |                         |                     | 20,20                      | 24-24                  |                  |                   | 4e-16                     | 2                      |                  |                   | 4e-41                  |               |         |                       |                         |                    |            |                   | 4e-41                            |
|         | END             |       |                    | 146                                       | 427                                       | 427               | · · · · ·            |                        |                     | 160                  | •                       |                     | 777                        |                        |                  |                   | 146                       | 2                      |                  |                   | 324                    |               |         |                       |                         |                    |            |                   | 323                              |
|         | START           |       |                    | 64                                        | 352                                       | 352               | 1                    |                        |                     | 63                   |                         |                     | 353                        | 700                    | ,                |                   | 23                        | 40                     |                  |                   | 151                    |               |         |                       |                         |                    |            |                   | 157                              |
|         | CHAIN           | }     |                    | A                                         | A                                         |                   |                      |                        |                     |                      |                         |                     |                            | Ą                      |                  |                   | <b>V</b>                  | ¢                      |                  |                   |                        |               |         |                       |                         |                    |            |                   |                                  |
|         | PDB             | }     |                    | 1d8z                                      | 1d9a                                      | 1 44              | 1111                 |                        |                     | 1fht                 |                         |                     | 15:1                       | /[17                   |                  |                   | 167                       | ) (tr                  | -                |                   | 1ha1                   |               |         |                       |                         |                    |            |                   | 1ha1                             |
|         | SEQ             | ġ     | 5                  | 1792                                      | 1792                                      | 1702              | 76/1                 |                        |                     | 1792                 |                         |                     | 0000                       | 76/1                   |                  |                   | 1702                      | 76/1                   |                  |                   | 1797                   | 7             |         |                       |                         |                    |            |                   | 1792                             |

| -       |                |            | ·                                |                                             |            |                   |                        |                           |                       |                         |                    |                                    |                        |               |         |                        |                         |                    |            | 7                 |                        | _             |         |                       |                         |                    |                               | T                         | l       |
|---------|----------------|------------|----------------------------------|---------------------------------------------|------------|-------------------|------------------------|---------------------------|-----------------------|-------------------------|--------------------|------------------------------------|------------------------|---------------|---------|------------------------|-------------------------|--------------------|------------|-------------------|------------------------|---------------|---------|-----------------------|-------------------------|--------------------|-------------------------------|---------------------------|---------|
|         | PDB annotation |            | NUCLEAR<br>RIBONUCLEOPROTEIN A1, | NUCLEAK PROTEIN, HINGIR,<br>PRD RRM RNP RNA | BINDING, 2 | RIBONUCLEOPROTEIN | NUCLEAR PROTEIN        | HEI EKUGENEUUS<br>NUCLEAR | RIBONUCLEOPROTEIN A1, | NUCLEAR PROTEIN, HNRNP, | RBD, RRM, RNP, KNA | BINDING, 2<br>RIBONI ICI EOPROTEIN | NUCLEAR PROTEIN        | HETEROGENEOUS | NUCLEAR | KIBONUCLEUPKUI EIN AI, | NUCLEAR PROTEIN, HNRNP, | RBD, RRM, RNP, RNA | BINDING, 2 | KIBONUCLEUFROILIN | NUCLEAR PROJEIN        | HEIEROGENEOUS | NUCLEAR | RIBONUCLEOPROTEIN A1, | NUCLEAR PROTEIN, HNRNP, | RBD, RRM, RNP, RNA | BINDING, 2 RIBONICI EOPROTEIN |                           |         |
|         | Compound       |            |                                  |                                             |            |                   | HNRNP A1; CHAIN: NULL; |                           |                       |                         |                    |                                    | HNRNP A1; CHAIN: NULL; |               |         |                        |                         |                    |            |                   | HNRNP A1; CHAIN: NULL; |               |         |                       |                         |                    |                               | RIBONUCLEOPROTEIN PROTEIN |         |
| Table 5 | SEQ            | FOLD score |                                  |                                             |            | •                 |                        |                           |                       |                         |                    |                                    |                        |               |         |                        |                         |                    |            |                   |                        |               |         |                       |                         |                    |                               |                           |         |
| Tab     | PMF            | score      |                                  |                                             |            |                   | 1.00                   |                           |                       |                         |                    |                                    | 1.00                   | )<br>)        |         |                        |                         |                    |            |                   | 0.09                   |               |         |                       |                         |                    |                               | 1.00                      | >>>     |
|         | Verify         | score      |                                  |                                             |            |                   | 0.46                   |                           |                       |                         |                    |                                    | 0.85                   | 9             |         |                        |                         |                    |            |                   | 0.07                   |               |         |                       |                         |                    |                               | -0.09                     | 10.0    |
|         | Psi            | Blast      |                                  |                                             |            |                   | 1.6e-38                |                           |                       |                         |                    |                                    | 1 26-31                | 1.50          |         |                        |                         |                    |            |                   | 1.5e-35                |               |         |                       |                         |                    |                               | 1 8e-20                   | 1.00-40 |
|         | END            | AA         |                                  |                                             |            |                   | 425                    |                           |                       |                         | ,                  |                                    | 425                    | 7             |         |                        |                         |                    |            |                   | 143                    |               |         |                       |                         |                    |                               | 427                       | 171     |
|         | START          | AA         |                                  |                                             |            |                   | 246                    |                           |                       |                         |                    |                                    | 248                    | 0+7           |         |                        |                         |                    |            |                   | 5                      |               |         |                       |                         |                    |                               | 352                       | 777     |
|         | CHAIN          | <u> </u>   |                                  |                                             |            |                   |                        | 10 10 10 10               |                       |                         |                    |                                    |                        |               |         | _                      |                         |                    |            |                   |                        |               |         |                       |                         |                    |                               | <                         | A       |
|         | PDB            | <u></u>    |                                  |                                             |            |                   | 1ha1                   |                           |                       |                         |                    |                                    | 1101                   | I III I       |         |                        |                         |                    |            |                   | 1ha1                   |               |         |                       |                         |                    |                               | 1                         | Inrc    |
|         | SEQ            | A 5        | NO.                              |                                             |            |                   | 1792                   |                           |                       |                         |                    |                                    | 1702                   | 76/1          |         |                        |                         |                    | •          |                   | 1792                   |               |         |                       |                         |                    |                               | 1707                      | 1/92    |

|         | PDB annotation |       |                                                                             |                                                                                        | ding I driftly agon to the court | KIBONUCLEOPROTEIN FIB, PTB-C198,                    | HETEROGENEOUS | NUCLEAR<br>POI VEVERAMENTE TEACT | BINDING PROTEIN, RNP. | RNA, SPICING, 2 | TRANSLATION | RIBONUCLEOPROTEIN PTB, | PIB-C198,<br>HETEROGENEOUS | NUCLEAR | POLYPYRIMIDINE TRACT | BINDING PROTEIN, RNP, | RNA, SPICING, 2 | TRANSLATION |                          |                         |                             |                                |                            |                       |                          |
|---------|----------------|-------|-----------------------------------------------------------------------------|----------------------------------------------------------------------------------------|----------------------------------|-----------------------------------------------------|---------------|----------------------------------|-----------------------|-----------------|-------------|------------------------|----------------------------|---------|----------------------|-----------------------|-----------------|-------------|--------------------------|-------------------------|-----------------------------|--------------------------------|----------------------------|-----------------------|--------------------------|
|         | Compound       |       | FROM UI SMALL NUCLEAR<br>RIBONUCLEOPROTEIN (SNRNP<br>UI) INRC 3 (N-TERMINAL | FRAGMENT, RESIDUES 1 - 95)<br>MUTANT WITH GLN 85 INRC 4<br>REPLACED BY CYS (Q85C) INRC | 5                                | POLYPYRIMIDINE TRACT-<br>BINDING PROTEIN; CHAIN: A; |               |                                  |                       |                 |             | POLYPYRIMIDINE TRACT-  | BINDING PROTEIN; CHAIN: A; |         |                      |                       |                 |             | RNA-BINDING PROTEIN SEX- | TEPMINIS OF SECOND RNA. | BINDING DOMAIN 18XL 3 (RBD- | 2), RESIDUES 199 - 294 PLUS N- | TERMINAL MET) 1SXL 4 (NMR, | 17 STRUCTURES) 1SXL 5 | RNA-BINDING PROTEIN SEX- |
| Table 5 | SEQ            | FOLD  | -                                                                           | -                                                                                      |                                  |                                                     |               |                                  |                       |                 |             |                        |                            |         |                      |                       |                 |             | 55.90                    |                         |                             |                                |                            |                       |                          |
| Tab     | PMF            | score |                                                                             |                                                                                        |                                  | 0.99                                                |               |                                  |                       |                 |             | 0.74                   | ,                          |         |                      |                       |                 |             |                          |                         |                             |                                |                            |                       | 1.00                     |
|         | Verify         | score |                                                                             |                                                                                        |                                  | 0.44                                                |               |                                  |                       |                 |             | 0.19                   |                            |         |                      |                       |                 |             |                          |                         |                             |                                |                            |                       | 0.78                     |
|         | Psi            | Blast |                                                                             |                                                                                        |                                  | 4e-40                                               |               |                                  |                       |                 |             | 1.6e-39                |                            |         |                      |                       |                 |             | 2e-20                    |                         |                             |                                |                            |                       | 2e-20                    |
|         | END            | AA    |                                                                             |                                                                                        |                                  | 327                                                 |               |                                  |                       |                 |             | 426                    |                            |         |                      |                       |                 |             | 428                      |                         |                             |                                |                            |                       | 427                      |
|         | START          | AA    |                                                                             |                                                                                        |                                  | 157                                                 | 4.            |                                  |                       |                 |             | 248                    |                            |         |                      |                       |                 |             | 339                      |                         | ,                           |                                |                            |                       | 349                      |
|         | CHAIN          | О     |                                                                             |                                                                                        |                                  | A                                                   |               |                                  |                       |                 |             | A                      |                            |         |                      |                       |                 |             |                          |                         |                             |                                |                            |                       |                          |
|         | PDB            | А     | -                                                                           |                                                                                        |                                  | Iqm9                                                |               | -                                |                       |                 |             | 1qm9                   |                            |         |                      |                       |                 |             | 1sxl                     |                         |                             |                                |                            |                       | 1sx1                     |
|         | SEO            | í e Ś |                                                                             |                                                                                        |                                  | 1792                                                |               |                                  |                       |                 |             | 1792                   |                            |         |                      |                       |                 |             | 1792                     |                         |                             |                                |                            |                       | 1792                     |

|         | PDB annotation |       |                                                |                             |                                                             |                       |                                                |                          |                             |                                |                                                   | COMPLEX                   | (RIBONUCLEOPROTEIN/RNA        |                        |                           | IN NOW DIRECTOR ATTE           | KNA-BINDING DOMAIN<br>RNA-BINDING DOMAIN | ALTERNATIVE SPLICING | RNA-BINDING PROTEIN        | SPLICING, U2 SNRNP, RBD,<br>RNA-BINDING PROTEIN | COMPLEX               | (RIBONUCLEOPROTEIN/DN | A) HNRNP A1, UP1;       | COMPLEX         | (RIBONUCLEOPROTEIN/DN     | NUCLEAR 2 |
|---------|----------------|-------|------------------------------------------------|-----------------------------|-------------------------------------------------------------|-----------------------|------------------------------------------------|--------------------------|-----------------------------|--------------------------------|---------------------------------------------------|---------------------------|-------------------------------|------------------------|---------------------------|--------------------------------|------------------------------------------|----------------------|----------------------------|-------------------------------------------------|-----------------------|-----------------------|-------------------------|-----------------|---------------------------|-----------|
|         | Compound       |       | LETHAL PROTEIN (C-<br>TERMINUS, OR SECOND RNA- | BINDING DOMAIN 1SXL 3 (RBD- | 2), RESIDUES 199 - 294 PLUS N-<br>TERMINAL MET) 1SXL 4 (NMR | 17 STRUCTURES) 1SXL 5 | RNA-BINDING PROTEIN SEX-<br>LETHAL PROTEIN (C- | TERMINUS, OR SECOND RNA- | BINDING DOMAIN 18XL 3 (RBD- | 2), RESIDUES 199 - 294 PLUS N- | TERMINAL MET) 1SXL 4 (NMR, 17 STRIICTURES) 1SXL 5 | U1A SPLICEOSOMAL PROTEIN; | 1URN 5 CHAIN: A, B, C; 1URN 6 | RNA 21MER HAIRPIN (5'- | (AP*AP*UP*CP*CP*AP*UP*UP* | IUKN II CHAIN: F, Q, R IUKN IS | SEX-LETHAL PROTEIN; CHAIN:               | MOLE,                | SPLICING FACTOR U2AF 65 KD | SUBUNIT; CHAIN: A;                              | HETEROGENEOUS NUCLEAR | RIBONUCLEOPROTEIN A1; | CHAIN: A; 12-NUCLEOTIDE | SINGLE-STRANDED | TELOMETRIC DNA; CHAIN: B; |           |
| Table 5 | SEQ            | FOLD  |                                                |                             |                                                             |                       |                                                |                          |                             |                                |                                                   |                           |                               |                        |                           |                                |                                          |                      |                            |                                                 | 98.66                 |                       |                         |                 |                           |           |
| Ta      | PMF            | score |                                                |                             |                                                             |                       | 0.49                                           |                          |                             |                                |                                                   | 1.00                      |                               |                        |                           |                                | 1.00                                     |                      | 1.00                       | - 11                                            |                       |                       |                         |                 |                           |           |
|         | Verify         | score |                                                |                             |                                                             |                       | -0.03                                          |                          |                             |                                |                                                   | 1.14                      |                               |                        |                           |                                | 98.0                                     |                      | 1.32                       |                                                 |                       | _                     |                         |                 |                           |           |
|         | Psi            | Blast |                                                |                             |                                                             | _                     | 1.2e-16                                        |                          |                             |                                |                                                   | 1.2e-20                   |                               |                        |                           |                                | 8e-22                                    |                      | 2e-20                      |                                                 | 8e-44                 | ·<br>·                |                         |                 |                           |           |
|         | END            | AA    |                                                |                             |                                                             |                       | 131                                            |                          |                             | =                              |                                                   | 427                       | į                             |                        |                           |                                | 426                                      |                      | 426                        |                                                 | 332                   | 1                     |                         |                 |                           |           |
|         | START          | AA    |                                                |                             |                                                             |                       | 56                                             |                          |                             |                                |                                                   | 352                       | 1                             |                        |                           |                                | 352                                      |                      | 352                        |                                                 | 151                   |                       |                         |                 |                           |           |
|         | CHAIN          |       |                                                |                             |                                                             |                       |                                                |                          |                             |                                |                                                   | A                         | 47                            |                        |                           |                                |                                          |                      | A                          |                                                 | 4                     | 1.                    |                         |                 |                           |           |
|         | PDB            | А     |                                                |                             | -                                                           |                       | 1sxl                                           |                          |                             |                                |                                                   | 11m                       |                               |                        |                           |                                | 2sxl                                     |                      | 2u2f                       |                                                 | Jun1                  | rdny                  |                         |                 |                           |           |
|         | SEQ            | A Š   |                                                |                             |                                                             |                       | 1792                                           |                          |                             |                                |                                                   | 1702                      | 7()1                          |                        |                           |                                | 1792                                     |                      | 1792                       | 1                                               | 1702                  | 7/11                  |                         |                 |                           |           |

(RIBONUCLEOPROTEIN/DN A), HETEROGENEOUS

(RIBONUCLEOPROTEIN/DN

A) HNRNP A1, UP1;

COMPLEX

SINGLE-STRANDED TELOMETRIC DNA; CHAIN: B;

CHAIN: A; 12-NUCLEOTIDE RIBONUCLEOPROTEIN A1;

RIBONUCLEOPROTEIN A1

COMPLEX

HETEROGENEOUS NUCLEAR

1.00

0.70

5.1e-33

425

248

K

2up1

1792

1792

A), HETEROGENEOUS NUCLEAR 2

|         | PDB annotation  | RIBONUCLEOPROTEIN A1 | COMPLEX               | (RIBONUCLEOPROTEIN/DN A) HNRNP A1, UP1;         | COMPLEX         | (RIBONUCLEOPROTEIN/DN     | A), HETEROGENEOUS | NUCLEAR 2 | RIBONUCLEOPROTEIN A1 | COMPLEX               | (RIBONUCLEOPROTEIN/DN | A) HNRNP A1, UP1;       | COMPLEX         | (RIBONUCLEOPROTEIN/DN     | A), HETEROGENEOUS | NUCLEAR 2 | RIBONUCLEOPROTEIN A1 | COMPLEX               | (RIBONUCLEOPROTEIN/DN | A) HNRNP A1, UP1;       | COMPLEX         | (RIBONUCLEOPROTEIN/DN     |
|---------|-----------------|----------------------|-----------------------|-------------------------------------------------|-----------------|---------------------------|-------------------|-----------|----------------------|-----------------------|-----------------------|-------------------------|-----------------|---------------------------|-------------------|-----------|----------------------|-----------------------|-----------------------|-------------------------|-----------------|---------------------------|
|         | Compound        |                      | HETEROGENEOUS NUCLEAR | RIBONUCLEOPROTEIN A1;<br>CHAN: A: 12-NUCLEOTIDE | SINGLE-STRANDED | TELOMETRIC DNA; CHAIN: B; |                   |           |                      | HETEROGENEOUS NUCLEAR | RIBONUCLEOPROTEIN A1; | CHAIN: A; 12-NUCLEOTIDE | SINGLE-STRANDED | TELOMETRIC DNA; CHAIN: B; |                   |           |                      | HETEROGENEOUS NUCLEAR | RIBONUCLEOPROTEIN A1; | CHAIN: A; 12-NUCLEOTIDE | SINGLE-STRANDED | TELOMETRIC DNA; CHAIN: B; |
| Table 5 | SEQ<br>FOLD     | 30010                |                       |                                                 |                 |                           |                   |           |                      |                       |                       |                         |                 |                           |                   |           |                      |                       |                       |                         |                 |                           |
| Ta      | PMF             |                      | 1.00                  |                                                 |                 |                           |                   |           |                      | 1.00                  |                       |                         |                 |                           |                   |           |                      | 1.00                  | ·                     |                         |                 |                           |
|         | Verify<br>score |                      | 1.00                  |                                                 |                 |                           |                   |           |                      | 1.00                  |                       |                         |                 |                           |                   |           |                      | 0.81                  |                       |                         |                 |                           |
|         | Psi<br>Blast    |                      | 1.7e-36               |                                                 |                 |                           |                   |           |                      | 8e-44                 |                       |                         |                 |                           |                   |           |                      | 6e-44                 |                       |                         |                 |                           |
|         | END             |                      | 333                   |                                                 |                 |                           |                   |           |                      | 330                   |                       |                         |                 |                           |                   |           |                      | 426                   |                       |                         |                 |                           |
|         | START           |                      | 156                   |                                                 |                 |                           |                   |           |                      | 157                   |                       |                         |                 |                           |                   |           |                      | 243                   |                       |                         |                 |                           |
|         | CHAIN<br>ID     |                      | A                     |                                                 |                 |                           |                   | -         |                      | A                     |                       |                         |                 |                           |                   |           |                      | A                     |                       |                         |                 |                           |
|         | PDB             |                      | 2up1                  |                                                 |                 |                           |                   |           |                      | Jun1                  |                       |                         |                 |                           |                   |           |                      | 2un1                  | 4                     |                         |                 |                           |
|         |                 |                      |                       |                                                 |                 |                           |                   |           |                      | 1                     |                       |                         |                 |                           |                   |           |                      | - 1                   |                       |                         |                 |                           |

1792

1792

SEQ NO:

|         | PDB annotation |        | NUCLEAR 2<br>RIBONUCLEOPROTEIN A1 | COMPLEX               | (RIBONUCLEOPROTEIN/DN | A) HNRNP A1, UP1;       | COMPLEX         | (RIBONUCLEOPROTEIN/DN     | A), HETEROGENEOUS | NUCLEAR 2 | RIBONUCLEOPROTEIN A1 | RNA BINDING DOMAIN RNA      | BINDING DOMAIN, RBD, | RNA RECOGNITION MOTIF, | RRM, 2 SPLICING | INHIBITOR, | TRANSLATIONAL | INHIBITOR, SEX 3 | DETERMINATION, X | CHROMOSOME DOSAGE | COMPENSATION | RNA BINDING DOMAIN RNA      | BINDING DOMAIN, RBD, | RNA RECOGNITION MOTIF, | RRM, 2 SPLICING | INHIBITOR, | TRANSLATIONAL | INHIBITOR, SEX 3 | DETERMINATION, X | CHROMOSOME DOSAGE | COMPENSATION | KNA BINDING DOMAIN KNA      |
|---------|----------------|--------|-----------------------------------|-----------------------|-----------------------|-------------------------|-----------------|---------------------------|-------------------|-----------|----------------------|-----------------------------|----------------------|------------------------|-----------------|------------|---------------|------------------|------------------|-------------------|--------------|-----------------------------|----------------------|------------------------|-----------------|------------|---------------|------------------|------------------|-------------------|--------------|-----------------------------|
|         | Compound       |        |                                   | HETEROGENEOUS NUCLEAR | RIBONUCLEOPROTEIN A1; | CHAIN: A; 12-NUCLEOTIDE | SINGLE-STRANDED | TELOMETRIC DNA; CHAIN: B; |                   |           |                      | SEX-LETHAL; CHAIN: A, B, C; |                      |                        |                 |            |               |                  |                  |                   |              | SEX-LETHAL; CHAIN: A, B, C; |                      |                        |                 |            |               |                  |                  |                   |              | SEX-LETHAL; CHAIN: A, B, C; |
| Table 5 | SEQ            | score  |                                   |                       |                       |                         |                 |                           |                   |           |                      |                             |                      |                        |                 |            |               |                  |                  |                   |              | 93.55                       |                      |                        |                 |            |               |                  |                  |                   |              |                             |
| Tat     | PMF            | score  |                                   | 0.18                  |                       |                         |                 |                           |                   |           |                      | 1.00                        |                      |                        |                 |            |               |                  |                  |                   |              |                             |                      |                        |                 |            |               |                  |                  |                   |              | 1.00                        |
|         | Verify         | score  |                                   | -0.05                 |                       |                         |                 |                           |                   |           |                      | 0.84                        |                      |                        |                 |            |               |                  |                  |                   |              |                             |                      |                        |                 |            |               |                  |                  |                   |              | 0.77                        |
|         | Psi            | Blast  |                                   | 1.2e-37               |                       |                         |                 |                           |                   |           |                      | 1.7e-23                     |                      |                        |                 |            |               |                  |                  |                   |              | 8e-43                       |                      |                        |                 |            |               |                  |                  |                   |              | 8e-43                       |
|         | END            | AA     |                                   | 150                   |                       |                         |                 |                           |                   |           |                      | 313                         |                      |                        |                 |            |               |                  |                  |                   |              | 318                         |                      |                        |                 |            |               |                  |                  |                   |              | 316                         |
|         | START          | AA<br> |                                   | 5                     |                       | 7.                      |                 |                           |                   |           |                      | 155                         |                      |                        |                 |            |               |                  |                  |                   |              | 156                         |                      |                        |                 |            |               |                  |                  |                   |              | 157                         |
|         | CHAIN          | 3      |                                   | <br> <br>             | •                     |                         |                 |                           |                   |           |                      | A                           |                      |                        |                 |            |               |                  |                  |                   |              | A                           | ·                    |                        |                 |            |               |                  |                  |                   |              | A                           |
|         | PDB            | <br>_  |                                   | 2up1                  | di<br>i               |                         |                 |                           |                   |           |                      | 3sxl                        |                      |                        |                 |            |               |                  |                  |                   |              | 3ex1                        |                      |                        |                 |            |               |                  |                  |                   |              | 3sx1                        |
|         | SEQ            | A S    |                                   | 1792                  | 7                     |                         |                 |                           |                   |           |                      | 1792                        |                      |                        |                 |            |               |                  |                  |                   |              | 1707                        | 7/11                 |                        |                 |            |               |                  |                  |                   |              | 1792                        |

|         | PDB annotation       | BINDING DOMAIN, RBD, RNA RECOGNITION MOTIF, RRM, 2 SPLICING INHIBITOR, TRANSLATIONAL INHIBITOR, SEX 3 DETERMINATION, X CHROMOSOME DOSAGE COMPENSATION | RNA BINDING DOMAIN RNA BINDING DOMAIN, RBD, RNA 2 SPLICING INHIBITOR, TRANSLATIONAL INHIBITOR, SEX 3 DETERMINATION, X CHROMOSOME DOSAGE COMPENSATION | LIM DOMAIN CONTAINING<br>PROTEINS LIM DOMAIN<br>CONTAINING PROTEINS,<br>METAL-BINDING PROTEIN,<br>ZINC 2 FINGER | LIM DOMAIN CONTAINING<br>PROTEINS LIM DOMAIN<br>CONTAINING PROTEINS,<br>METAL-BINDING PROTEIN,<br>ZINC 2 FINGER | LIM DOMAIN CONTAINING      |
|---------|----------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------|----------------------------|
|         | Compound             |                                                                                                                                                       | SEX-LETHAL; CHAIN: A, B, C;                                                                                                                          | QCRP2 (LIM1); CHAIN: NULL;                                                                                      | QCRP2 (LIMI); CHAIN: NULL;                                                                                      | QCRP2 (LIM1); CHAIN: NULL; |
| Table 5 | SEQ<br>FOLD<br>score |                                                                                                                                                       |                                                                                                                                                      |                                                                                                                 | 50.26                                                                                                           |                            |
| Tat     | PMF                  |                                                                                                                                                       | 1.00                                                                                                                                                 | 0.45                                                                                                            |                                                                                                                 | 0.53                       |
|         | Verify<br>score      |                                                                                                                                                       | 0.63                                                                                                                                                 | -0.04                                                                                                           |                                                                                                                 | 0.02                       |
|         | Psi<br>Blast         |                                                                                                                                                       | 6e-40                                                                                                                                                | 6.8e-16                                                                                                         | 4.8e-19                                                                                                         | 4.8e-19                    |
|         | END                  | -                                                                                                                                                     | 418                                                                                                                                                  | 62                                                                                                              | 09                                                                                                              | 59                         |
|         | START<br>AA          |                                                                                                                                                       | 248                                                                                                                                                  | ٤ .                                                                                                             | 4                                                                                                               | 5                          |
|         | CHAIN                |                                                                                                                                                       | ⋖                                                                                                                                                    |                                                                                                                 |                                                                                                                 |                            |
|         | PDB<br>ID            |                                                                                                                                                       | 3sxl                                                                                                                                                 | 1a7i                                                                                                            | 1a7i                                                                                                            | 1a7i                       |
|         | S E S                |                                                                                                                                                       | 1792                                                                                                                                                 | 1807                                                                                                            | 1807                                                                                                            | 1807                       |

|         | PDB annotation       | PROTEINS LIM DOMAIN<br>CONTAINING PROTEINS,<br>METAL-BINDING PROTEIN,<br>ZINC 2 FINGER | TRANSFERASE<br>TRANSFERASE, SH3<br>DOMAIN, NEBULIN, Z-DISK<br>ASSEMBLY, 2 ACTIN-<br>BINDING | TRANSFERASE<br>TRANSFERASE, SH3<br>DOMAIN, NEBULIN, Z-DISK<br>ASSEMBLY, 2 ACTIN-<br>BINDING | TRANSFERASE TRANSFERASE, SH3 DOMAIN, NEBULIN, Z-DISK ASSEMBLY, 2 ACTIN- BINDING | TRANSFERASE IL-2- INDUCIBLE T-CELL KINASE; TRANSFERASE, REGULATORY INTRAMOLECULAR COMPLEX, KINASE | TRANSFERASE IL-2- INDUCIBLE T-CELL KINASE; TRANSFERASE, REGULATORY INTRAMOLECULAR COMPLEX, KINASE |
|---------|----------------------|----------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------|
|         | Compound             |                                                                                        | NEBULIN; CHAIN: NULL;                                                                       | NEBULIN; CHAIN: NULL;                                                                       | NEBULIN; CHAIN: NULL;                                                           | ITK; CHAIN: NULL;                                                                                 | ITK; CHAIN: NULL;                                                                                 |
| Table 5 | SEQ<br>FOLD<br>score |                                                                                        | 80.79                                                                                       |                                                                                             |                                                                                 |                                                                                                   |                                                                                                   |
| Tat     | PMF                  |                                                                                        |                                                                                             | 1.00                                                                                        | 1.00                                                                            | 0.41                                                                                              | 0.45                                                                                              |
|         | Verify<br>score      |                                                                                        |                                                                                             | 0.56                                                                                        | 0.42                                                                            | 0.20                                                                                              | 0.31                                                                                              |
|         | Psi<br>Blast         |                                                                                        | 1e-18                                                                                       | 1e-18                                                                                       | 1.2e-13                                                                         | 8.5e-12                                                                                           | 7.2e-17                                                                                           |
|         | END                  |                                                                                        | 225                                                                                         | 225                                                                                         | 225                                                                             | 221                                                                                               | 223                                                                                               |
|         | START<br>AA          |                                                                                        | 166                                                                                         | 166                                                                                         | 168                                                                             | 151                                                                                               | 153                                                                                               |
|         | CHAIN                |                                                                                        |                                                                                             |                                                                                             |                                                                                 |                                                                                                   |                                                                                                   |
|         | PDB<br>ID            |                                                                                        | lark                                                                                        | 1ark                                                                                        | lark                                                                            | lawj                                                                                              | lawj                                                                                              |
|         | SEQ<br>D S           |                                                                                        | 1807                                                                                        | 1807                                                                                        | 1807                                                                            | 1807                                                                                              | 1807                                                                                              |

|         | PDB annotation |         | CONTRACTILE LIM DOMAIN, CRP, NMR, MUSCLE DIFFERENTIATION, CONTRACTILE | METAL-BINDING PROTEIN<br>LIM DOMAIN CONTAINING<br>PROTEINS ICTL 15 | SIGNALING PROTEIN LIM<br>DOMAIN CONTAINING<br>PROTEINS, METAL-BINDING<br>PROTEIN | SIGNALING PROTEIN LIM<br>DOMAIN CONTAINING<br>PROTEINS, METAL-BINDING<br>PROTEIN | SIGNALING PROTEIN LIM DOMAIN CONTAINING PROTEINS, METAL-BINDING PROTEIN | COMPLEX (SH3 DOMAIN/URAL ENHANCER) SRC- HOMOLOGY 3 DOMAIN; COMPLEX (SH3 DOMAIN/URAL ENHANCER), PROTO- ONCOGENE, 2 TRANSFERASE, TYROSINE- PROTEIN KINASE, PHOSPHORYLATION, 3 AIDS, MYRISTYLATION, |
|---------|----------------|---------|-----------------------------------------------------------------------|--------------------------------------------------------------------|----------------------------------------------------------------------------------|----------------------------------------------------------------------------------|-------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
|         | Compound       |         | CRP1; CHAIN: A;                                                       | AVIAN CYSTEINE RICH<br>PROTEIN; 1CTL 3                             | CYSTEINE AND GLYCINE-RICH<br>PROTEIN CRP2; CHAIN: A;                             | CYSTEINE AND GLYCINE-RICH<br>PROTEIN CRP2; CHAIN: A;                             | CYSTEINE AND GLYCINE-RICH<br>PROTEIN CRP2; CHAIN: A;                    | FYN TYROSINE KINASE; CHAIN:<br>A, C; HIV-1 NEF PROTEIN;<br>CHAIN: B, D;                                                                                                                          |
| Table 5 | SEQ            | FOLD    |                                                                       |                                                                    | 52.57                                                                            |                                                                                  |                                                                         |                                                                                                                                                                                                  |
| Tal     | PMF            | score   | 0.72                                                                  | 69:0                                                               |                                                                                  | 0.80                                                                             | 0.76                                                                    | 1.00                                                                                                                                                                                             |
|         | Verify         | score   | 80.0-                                                                 | -0.14                                                              |                                                                                  | 0.38                                                                             | 0.27                                                                    | 89.0                                                                                                                                                                                             |
|         | Psi            | Blast   | 8.5e-22                                                               | 8.5e-22                                                            | 1.2e-19                                                                          | 1.7e-18                                                                          | 1.2e-19                                                                 | 5.1e-20                                                                                                                                                                                          |
|         | END            | AA      | 74                                                                    | 74                                                                 | 09                                                                               | 09                                                                               | 59                                                                      | 225                                                                                                                                                                                              |
|         | START          | AA      | 5                                                                     | 5                                                                  | 2                                                                                | 2                                                                                | m                                                                       | 171                                                                                                                                                                                              |
|         | CHAIN          |         | A                                                                     |                                                                    | A                                                                                | A                                                                                | A                                                                       | ∀                                                                                                                                                                                                |
|         | PDB            | <u></u> | 1b8t                                                                  | 1ctl                                                               | 1cxx                                                                             | 1cxx                                                                             | 1cxx                                                                    | lefn                                                                                                                                                                                             |
|         | SEQ            | í A Ś   |                                                                       | 1807                                                               | 1807                                                                             | 1807                                                                             | 1807                                                                    | 1807                                                                                                                                                                                             |

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|         | PDB annotation       | GTP-BINDING, ATP-<br>BINDING, SH3 DOMAIN, 4<br>SH2 DOMAIN, PPII HELIX,<br>PXXP MOTIF | PHOSPHOTRANSFERASE C-SRC, P60-SRC; SRC, TYROSINE KINASE, PHOSPHORYLATION, SH2, SH3, 2 PHOSPHOTYROSINE, PROTO-ONCOGENE, PHOSPHOTRANSFERASE | TRANSFERASE PROTO- ONCOGENE TYROSINE KINASE; PROTO- ONCOGENE, TRANSFERASE, TYROSINE-PROTEIN KINASE, 2 PHOSPHORYLATION, ATP- BINDING, MYRISTYLATION, SH3 DOMAIN, 3 COMPLEX (PHOSPHOTRANSFERASE/PE PTUDE) |                                                                                                                                                             | SIGNAL TRANSDUCTION<br>ADAPTOR SH2, SH3 1GRI 14       |
|---------|----------------------|--------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------|
|         | Compound             |                                                                                      | TYROSINE-PROTEIN KINASE<br>SRC; CHAIN: NULL;                                                                                              | PHOSPHOTRANSFERASE FYN;<br>CHAIN: A; 3BP-2; CHAIN: B;                                                                                                                                                   | ADAPTOR PROTEIN CONTAINING SH2 AND SH3 GROWTH FACTOR RECEPTOR- BOUND PROTEIN 2 (GRB2) 1GFC 3 (C-TERMINAL SH3 DOMAIN) (NMR, MINIMIZED MEAN STRUCTURE) 1GFC 4 | GROWTH FACTOR BOUND<br>PROTEIN 2; 1GRI 5 CHAIN: A, B; |
| Table 5 | SEQ<br>FOLD<br>score |                                                                                      |                                                                                                                                           |                                                                                                                                                                                                         |                                                                                                                                                             |                                                       |
| Tat     | PMF                  |                                                                                      | 1.00                                                                                                                                      | 66.0                                                                                                                                                                                                    | 1.00                                                                                                                                                        | 0.99                                                  |
|         | Verify<br>score      |                                                                                      | 0.27                                                                                                                                      | 0.54                                                                                                                                                                                                    | 09.0                                                                                                                                                        | 69.0                                                  |
|         | Psi<br>Blast         |                                                                                      | 5.1e-19                                                                                                                                   | 1e-20                                                                                                                                                                                                   | 6.8e-19                                                                                                                                                     | 3.4e-19                                               |
|         | END<br>AA            |                                                                                      | 224                                                                                                                                       | 225                                                                                                                                                                                                     | 225                                                                                                                                                         | 225                                                   |
|         | START                |                                                                                      | 168                                                                                                                                       | 166                                                                                                                                                                                                     | 167                                                                                                                                                         | 165                                                   |
|         | CHAIN                |                                                                                      |                                                                                                                                           | ⋖                                                                                                                                                                                                       |                                                                                                                                                             | А                                                     |
|         | PDB<br>ID            |                                                                                      | 1 fink                                                                                                                                    | 1fyn                                                                                                                                                                                                    | 1gfc                                                                                                                                                        | 1gri                                                  |
|         | SEQ                  |                                                                                      | 1807                                                                                                                                      | 1807                                                                                                                                                                                                    | 1807                                                                                                                                                        | 1807                                                  |

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|         | PDB annotation |          |        | SIGNAL TRANSDUCTION<br>ADAPTOR SH2, SH3 1GRI 14                 | SIGNAL TRANSDUCTION<br>ADAPTOR SH2, SH3 1GRI 14                 | METAL-BINDING PROTEIN<br>CRIP; METAL-BINDING<br>PROTEIN, LIM DOMAIN<br>PROTEIN | METAL-BINDING PROTEIN<br>CRIP; METAL-BINDING<br>PROTEIN, LIM DOMAIN<br>PROTEIN |                                                                                                           | METAL-BINDING PROTEIN<br>LIM DOMAIN, ZINC-FINGER,<br>METAL-BINDING PROTEIN | METAL-BINDING PROTEIN.<br>LIM DOMAIN, ZINC-FINGER,<br>METAL-BINDING PROTEIN | METAL-BINDING PROTEIN<br>LIM DOMAIN, ZINC-FINGER,<br>METAL-BINDING PROTEIN | PROTEIN KINASE CDK2;<br>PROTEIN KINASE, CELL       |
|---------|----------------|----------|--------|-----------------------------------------------------------------|-----------------------------------------------------------------|--------------------------------------------------------------------------------|--------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------|-----------------------------------------------------------------------------|----------------------------------------------------------------------------|----------------------------------------------------|
|         | Compound       |          | 1GRI 6 | GROWTH FACTOR BOUND<br>PROTEIN 2; 1GRI 5 CHAIN: A, B;<br>1GRI 6 | GROWTH FACTOR BOUND<br>PROTEIN 2; 1GRI 5 CHAIN: A, B;<br>1GRI 6 | CYSTEINE RICH INTESTINAL<br>PROTEIN; CHAIN: NULL;                              | CYSTEINE RICH INTESTINAL<br>PROTEIN; CHAIN: NULL;                              | PHOSPHOTRANSFERASE FYN<br>PROTO-ONCOGENE TYROSINE<br>KINASE (E.C.2.7.1.112) 1SHF 3<br>(SH3 DOMAIN) 1SHF 4 | LASP-1; CHAIN: NULL;                                                       | LASP-1; CHAIN: NULL;                                                        | LASP-1; CHAIN: NULL;                                                       | CYCLIN-DEPENDENT PROTEIN<br>KINASE 2; CHAIN: NULL; |
| Table 5 | SEQ            | FOLD     |        | 51.32                                                           |                                                                 | 55.79                                                                          |                                                                                |                                                                                                           |                                                                            | 56.91                                                                       |                                                                            |                                                    |
| Tal     | PMF            | score    |        |                                                                 | -0.18                                                           |                                                                                | 0.62                                                                           | 86.0                                                                                                      | 1.00                                                                       |                                                                             | 1.00                                                                       | 1.00                                               |
|         | Verify         | score    |        |                                                                 | 0.16                                                            |                                                                                | 0.32                                                                           | -0.17                                                                                                     | -0.54                                                                      |                                                                             | -0.54                                                                      | 0.58                                               |
|         | Psi            | Blast    |        | 4.8e-15                                                         | 4.8e-15                                                         | 1.2e-21                                                                        | 1.2e-21                                                                        | 1.7e-20                                                                                                   | 6.8e-09                                                                    | 8.4e-12                                                                     | 8.4e-12                                                                    | 0                                                  |
|         | END            | AA       |        | 225                                                             | 225                                                             | 73                                                                             | 75                                                                             | 225                                                                                                       | 30                                                                         | 30                                                                          | 30                                                                         | 367                                                |
|         | START          | AA       |        | 18                                                              | 49                                                              | ಣ                                                                              | ю                                                                              | 171                                                                                                       | 1                                                                          | 1                                                                           | -                                                                          | 70                                                 |
|         | CHAIN          |          |        | A                                                               | A                                                               |                                                                                |                                                                                | А                                                                                                         |                                                                            |                                                                             |                                                                            |                                                    |
|         | PDB            | <u>a</u> | -      | 1gri                                                            | 1gri                                                            | liml                                                                           | liml                                                                           | lshf                                                                                                      | 1zfo                                                                       | 1zfo                                                                        | 1zfo                                                                       | laql                                               |
|         | SEQ            | A 8      |        | 1807                                                            | 1807                                                            | 1807                                                                           | 1807                                                                           | 1807                                                                                                      | 1807                                                                       | 1807                                                                        | 1807                                                                       | 1808                                               |

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| 1       |                |          |                            |                       |                                  | T                        |                        |        |                       |                    | $\top$                         |                            |                          |                  |                         |                  |                     |                          |                |                    | T            |                            |                          |                  |                         |                  |                     |                          |                                      |
|---------|----------------|----------|----------------------------|-----------------------|----------------------------------|--------------------------|------------------------|--------|-----------------------|--------------------|--------------------------------|----------------------------|--------------------------|------------------|-------------------------|------------------|---------------------|--------------------------|----------------|--------------------|--------------|----------------------------|--------------------------|------------------|-------------------------|------------------|---------------------|--------------------------|--------------------------------------|
|         | PDB annotation |          | CYCLE,<br>PHOSPHORYLATION, | STAUROSPORINE, 2 CELL | DIVISION, MITOSIS,<br>INHIBITION | PROTEIN KINASE CDK2;     | PROTEIN KINASE, CELL   | CYCLE, | STAUROSPORINE, 2 CELL | DIVISION, MITOSIS, | INHIBITION                     | COMPLEX                    | (KINASE/INHIBITOR) CDK6; | PI9INK4D; CYCLIN | DEPENDENT KINASE,       | CYCLIN DEPENDENT | KINASE INHIBITORY 2 | PROTEIN, CDK, INK4, CELL | CYCLE, COMPLEX | (KINASE/INHIBITOR) | HEADER HELIX | COMPLEX                    | (KINASE/INHIBITOR) CDK6; | P19INK4D; CYCLIN | DEPENDENT KINASE,       | CYCLIN DEPENDENT | KINASE INHIBITORY 2 | PROTEIN, CDK, INK4, CELL | CYCLE, COMPLEX<br>(KINASE/INHIBITOR) |
|         | Compound       |          |                            |                       |                                  | CYCLIN-DEPENDENT PROTEIN | KINASE 2; CHAIN: NULL; |        |                       |                    | י מי נותנו מונותות ות ומיוסיוס | CYCLIN-DEPENDENT KINASE 6; | CHAIN: A, C; CYCLIN-     | DEPENDENT KINASE | INHIBITOR; CHAIN: B, D; |                  |                     |                          |                |                    |              | CYCLIN-DEPENDENT KINASE 6; | CHAIN: A, C; CYCLIN-     | DEPENDENT KINASE | INHIBITOR; CHAIN: B, D; |                  |                     |                          |                                      |
| Table 5 | SEQ            | FOLD     |                            |                       |                                  | 235.79                   |                        |        | ···                   |                    | 101                            | 18/.00                     |                          | ·                |                         |                  |                     |                          |                |                    |              |                            |                          |                  |                         |                  |                     |                          |                                      |
| Tal     | PMF            | score    |                            |                       |                                  |                          |                        |        |                       |                    |                                |                            |                          |                  |                         |                  |                     |                          |                |                    |              | 1.00                       |                          |                  |                         |                  |                     |                          |                                      |
|         | Verify         | score    |                            |                       |                                  |                          |                        |        |                       |                    |                                |                            |                          |                  |                         |                  |                     |                          |                |                    |              | 0.43                       |                          |                  |                         |                  |                     |                          |                                      |
|         | Psi            | Blast    |                            |                       |                                  | 0                        |                        |        |                       |                    | 7                              | 5.4e-90                    |                          |                  |                         |                  |                     |                          |                |                    |              | 3.4e-90                    |                          |                  |                         |                  |                     |                          |                                      |
|         | END            | AA       |                            |                       |                                  | 368                      |                        |        |                       |                    | 0,00                           | 328                        |                          |                  |                         |                  |                     |                          |                |                    |              | 358                        |                          |                  |                         |                  |                     |                          |                                      |
|         | START          | AA       |                            |                       |                                  | 70                       |                        |        |                       |                    |                                | /1                         |                          | •                |                         |                  |                     |                          |                |                    |              | 72                         |                          |                  |                         |                  |                     |                          |                                      |
|         | CHAIN          | <u> </u> |                            |                       |                                  |                          |                        |        |                       |                    |                                | Ą                          |                          |                  |                         |                  |                     |                          |                |                    |              | Ą                          |                          |                  |                         |                  |                     |                          |                                      |
|         | PDB            | <b>A</b> |                            |                       |                                  | laqi                     | 1                      |        |                       |                    |                                | 1018                       |                          |                  |                         |                  |                     |                          |                |                    |              | 1bi8                       |                          |                  |                         |                  |                     |                          |                                      |
|         | SEQ            | A &      |                            |                       |                                  | 1808                     |                        |        | _                     |                    | 0001                           | 1808                       |                          |                  |                         |                  |                     |                          |                |                    |              | 1808                       | <del>~~~</del>           |                  |                         |                  |                     |                          |                                      |

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| non constitution | FLUB annotation      | HEADER HELIX | COMPLEX (INHIBITOR PROTEIN/KINASE) INHIBITOR PROTEIN,       | CYCLIN-DEPENDENT<br>KINASE, CELL CYCLE 2 | CONTROL, ALPHA/BETA,<br>COMPLEX (INHIBITOR<br>PROTEIN/KINASE) | COMPLEX (INHIBITOR PROTEIN/KINASE)                          | INHIBITOR PROTEIN, | KINASE, CELL CYCLE 2 | CONTROL, ALPHA/BETA, | COMPLEX (INHIBITOR<br>PROTEIN/KINASE) |                                                      |                                                |                          |                          |                       | PROTEIN KINASE CDK2;   | SERINE/THREONINE       | PROTEIN KINASE, ATP- | CELL DIVISION, MITOSIS, |
|------------------|----------------------|--------------|-------------------------------------------------------------|------------------------------------------|---------------------------------------------------------------|-------------------------------------------------------------|--------------------|----------------------|----------------------|---------------------------------------|------------------------------------------------------|------------------------------------------------|--------------------------|--------------------------|-----------------------|------------------------|------------------------|----------------------|-------------------------|
|                  | Compound             |              | CYCLIN-DEPENDENT KINASE 6;<br>CHAIN: A; P19INK4D; CHAIN: B; |                                          |                                                               | CYCLIN-DEPENDENT KINASE 6;<br>CHAIN: A: P19INK4D: CHAIN: B: |                    |                      |                      |                                       | PHOSPHOTRANSFERASE CAMP-<br>DEPENDENT PROTEIN KINASE | CATALYTIC SUBUNIT 1CMK 3 (E.C.2.7.1.37) 1CMK 4 | PHOSPHOTRANSFERASE CAMP- | DEPENDENT PROTEIN KINASE | (E.C.2.7.1.37) 1CMK 4 | HUMAN CYCLIN-DEPENDENT | MINASE Z. CHAIN: NOLL, |                      |                         |
| Table 5          | SEQ<br>FOLD<br>score |              |                                                             |                                          |                                                               | 213.62                                                      |                    |                      |                      |                                       | 109.44                                               |                                                |                          |                          |                       |                        |                        |                      |                         |
| Tal              | FMF                  |              | 1.00                                                        |                                          |                                                               |                                                             |                    |                      |                      |                                       |                                                      |                                                | 89.0                     |                          |                       | 1.00                   |                        |                      |                         |
| 3. 1.            | Verity<br>score      |              | 69:0                                                        |                                          |                                                               |                                                             |                    |                      |                      |                                       |                                                      |                                                | 60.0                     |                          |                       | 0.70                   |                        |                      |                         |
|                  | Psı<br>Blast         |              | 5.1e-98                                                     |                                          |                                                               | 5.1e-98                                                     |                    |                      |                      |                                       | 6.8e-54                                              |                                                | 6.8e-54                  |                          |                       | 0                      |                        |                      |                         |
| į                | AA                   |              | 360                                                         |                                          |                                                               | 366                                                         |                    |                      |                      |                                       | 388                                                  |                                                | 391                      |                          |                       | 367                    |                        |                      |                         |
| THE THE          | START                |              | 29                                                          |                                          |                                                               | 89                                                          |                    |                      |                      |                                       | 21                                                   |                                                | 31                       |                          |                       | 70                     |                        |                      |                         |
| Iditio           | CHAIN                |              | A                                                           |                                          |                                                               | A                                                           |                    |                      |                      |                                       | H                                                    |                                                | Э                        |                          |                       |                        |                        |                      |                         |
| i<br>G           | PDB<br>ID            |              | 1blx                                                        |                                          |                                                               | 1blx                                                        |                    |                      |                      |                                       | 1cmk                                                 |                                                | 1cmk                     |                          |                       | 1hcl                   |                        |                      |                         |
| 040              |                      |              | 1808                                                        |                                          | ***                                                           | 1808                                                        |                    |                      |                      |                                       | 1808                                                 |                                                | 1808                     |                          |                       | 1808                   |                        |                      |                         |

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|         | PDB annotation  | PHOSPHORYLATION | PROTEIN KINASE CDK2;<br>TRANSFERASE,<br>SERINE/THREONINE | PROTEIN KINASE, ATP-<br>BINDING, 2 CELL CYCLE,<br>CELL DIVISION, MITOSIS,<br>PHOSPHORYLATION | TYROSINE KINASE<br>TYROSINE KINASE-<br>INHIBITOR COMPLEX | DOWN-REGULATED<br>KINASE, 2 ORDERED | ACTIVATION LOOP | TRANSFERASE MITOGEN ACTIVATED PROTEIN          | KINASE, MAP 2, ERK2; | TRANSFERASE, | PROTEIN KINASE MAP | KINASE, 2 ERK2 | TRANSFERASE MITOGEN     | ACITVATED PROTEIN KINASE MAP 2 FRK2 | TRANSFERASE, | SERINE/THREONINE- | PROTEIN KINASE, MAP | KINASE, 2 ERK2 | CON THE EW (ZPAIC)           | COMPLEX (ZINC)<br>FINGER/DNA) COMPLEX         |
|---------|-----------------|-----------------|----------------------------------------------------------|----------------------------------------------------------------------------------------------|----------------------------------------------------------|-------------------------------------|-----------------|------------------------------------------------|----------------------|--------------|--------------------|----------------|-------------------------|-------------------------------------|--------------|-------------------|---------------------|----------------|------------------------------|-----------------------------------------------|
|         | Compound        |                 | HUMAN CYCLIN-DEPENDENT<br>KINASE 2; CHAIN: NULL;         |                                                                                              | HAEMATOPOETIC CELL KINASE (HCK); CHAIN: A;               |                                     |                 | EXTRACELLULAR REGULATED KINASE 2; CHAIN: NULL; |                      |              |                    |                | EXTRACELLULAR REGULATED | KINASE 2; CHAIN: NULL;              |              |                   |                     |                | יימייימים מיוייים הנמיד מההה | QGSK ZINC FINGER PEPTIDE;<br>CHAIN: A; DUPLEX |
| Table 5 | SEQ<br>FOLD     |                 | 269.62                                                   |                                                                                              |                                                          |                                     |                 | 197.73                                         |                      |              |                    |                |                         |                                     |              |                   |                     |                |                              |                                               |
| Tal     | PMF             |                 |                                                          |                                                                                              | 96.0                                                     |                                     |                 |                                                |                      |              |                    |                | 1.00                    |                                     |              |                   |                     |                |                              | 0.33                                          |
|         | Verify<br>score |                 |                                                          |                                                                                              | 60.0                                                     |                                     |                 |                                                |                      |              | •                  |                | 0.53                    |                                     |              |                   |                     |                | 0                            | -0.50                                         |
|         | Psi<br>Blast    |                 | 0                                                        |                                                                                              | 1.4e-34                                                  |                                     |                 | 66-99                                          |                      |              |                    |                | 66-99                   |                                     |              |                   |                     |                | 1                            | 8.5e-25                                       |
|         | END<br>AA       |                 | 368                                                      |                                                                                              | 316                                                      |                                     |                 | 399                                            |                      |              |                    |                | 361                     |                                     |              |                   |                     |                |                              | 540                                           |
|         | START<br>AA     |                 | 70                                                       |                                                                                              | 51                                                       |                                     |                 | 95                                             |                      |              |                    |                | 29                      |                                     |              |                   |                     |                |                              | 462                                           |
|         | CHAIN<br>ID     |                 |                                                          |                                                                                              | A                                                        |                                     |                 |                                                |                      |              |                    |                |                         |                                     |              |                   |                     |                |                              | А                                             |
|         | PDB<br>ID       |                 | 1hc1                                                     |                                                                                              | 1qcf                                                     |                                     |                 | 3erk                                           |                      |              |                    |                | 3erk                    |                                     |              |                   |                     |                |                              | lalh                                          |
|         | SEQ<br>No.      | j<br>Z          | 1808                                                     |                                                                                              | 1808                                                     |                                     | -               | 1808                                           |                      |              |                    |                | 1808                    |                                     |              |                   |                     |                |                              | 1856                                          |

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| DDB onnotation | oration              | ZINC                                                      | EX<br>JINC<br>G                                                                                   | C<br>N<br>N                                                                                       | Z C                                                                                               | C<br>Z X                                                                                          | د<br>در                                                                                           | ي                                                                        |
|----------------|----------------------|-----------------------------------------------------------|---------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------|
| 10             | rub allık            | (ZINC FINGER/DNA), ZINC<br>FINGER, DNA-BINDING<br>PROTEIN | COMPLEX (ZINC<br>FINGER/DNA) COMPLEX<br>(ZINC FINGER/DNA), ZINC          |
| bustonmo       | Compound             | OLIGONUCLEOTIDE BINDING<br>SITE; CHAIN: B, C;             | QGSR ZINC FINGER PEPTIDE;<br>CHAIN: A; DUPLEX<br>OLIGONUCLEOTIDE BINDING<br>SITE; CHAIN: B, C;    | QGSR ZINC FINGER PEPTIDE;<br>CHAIN: A; DUPLEX<br>OLIGONUCLEOTIDE BINDING<br>SITE; CHAIN: B, C;    | QGSR ZINC FINGER PEPTIDE;<br>CHAIN: A; DUPLEX<br>OLIGONUCLEOTIDE BINDING<br>SITE; CHAIN: B, C;    | QGSR ZINC FINGER PEPTIDE;<br>CHAIN: A; DUPLEX<br>OLIGONUCLEOTIDE BINDING<br>SITE; CHAIN: B, C;    | QGSR ZINC FINGER PEPTIDE;<br>CHAIN: A; DUPLEX<br>OLIGONUCLEOTIDE BINDING<br>SITE; CHAIN: B, C;    | QGSR ZINC FINGER PEPTIDE;<br>CHAIN: A; DUPLEX<br>OLIGONUCLEOTIDE BINDING |
| Table 5        | SEQ<br>FOLD<br>score |                                                           |                                                                                                   |                                                                                                   |                                                                                                   |                                                                                                   |                                                                                                   | 75.25                                                                    |
| Ta             | score                |                                                           | 0.04                                                                                              | 0.64                                                                                              | 1.00                                                                                              | 0.95                                                                                              | 0.86                                                                                              |                                                                          |
| Vowifi.        | score                |                                                           | -0.53                                                                                             | -0.16                                                                                             | 0.13                                                                                              | -0.16                                                                                             | -0.00                                                                                             |                                                                          |
|                | rsi<br>Blast         |                                                           | 2e-14                                                                                             | 5.1e-29                                                                                           | 1.2e-30                                                                                           | 1.5e-30                                                                                           | 5.1e-30                                                                                           | 3.4e-31                                                                  |
| CIVII          | AA                   |                                                           | 572                                                                                               | 598                                                                                               | 979                                                                                               | 654                                                                                               | 682                                                                                               | 684                                                                      |
| CTABT          | SIAKI<br>AA          |                                                           | 495                                                                                               | 516                                                                                               | 546                                                                                               | 574                                                                                               | 602                                                                                               | 602                                                                      |
| CITABLE        | CHAIN                |                                                           | A                                                                                                 | ¥                                                                                                 | ٧                                                                                                 | ¥                                                                                                 | A                                                                                                 | А                                                                        |
| מטת            | PDB<br>ID            |                                                           | lalh                                                                                              | 1a1h                                                                                              | 1a1h                                                                                              | lalh                                                                                              | laih                                                                                              | la1h                                                                     |
| City           | A A S                |                                                           | 1856                                                                                              | 1856                                                                                              | 1856                                                                                              | 1856                                                                                              | 1856                                                                                              | 1856                                                                     |

|         | PDB annotation  | FINGER, DNA-BINDING<br>PROTEIN | COMPLEX (ZINC<br>FINGER/DNA) COMPLEX          | (ZINC FINGER/DNA), ZINC<br>FINGER, DNA-BINDING<br>PROTEIN |                                                                                                                                                        | GENE REGULATION POZ<br>DOMAIN; PROTEIN-             | PROTEIN INTERACTION DOMAIN. | TRANSCRIPTIONAL 2 | PROTEIN, X-RAY | CRYSTALLOGRAPHY, 3 | PROTEIN STRUCTURE, | PROMYELOCYTIC | LEUKEMIA, GENE<br>REGULATION | COMPLEX (ZINC           | FINGER/DNA) ZINC FINGER, | PROTEIN-DNA              | INTERACTION, PROTEIN | DESIGN, 2 CKTSTAL<br>STRUCTURE, COMPLEX |
|---------|-----------------|--------------------------------|-----------------------------------------------|-----------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------|-----------------------------|-------------------|----------------|--------------------|--------------------|---------------|------------------------------|-------------------------|--------------------------|--------------------------|----------------------|-----------------------------------------|
|         | Compound        | SITE, CHAIN: B, C;             | QGSR ZINC FINGER PEPTIDE;<br>CHAIN: A; DUPLEX | OLIGONUCLEOTIDE BINDING<br>SITE; CHAIN: B, C;             | DNA-BINDING PROTEIN<br>HUMAN ENHANCER-BINDING<br>PROTEIN MBP-1 MUTANT WITH<br>CYS 11 1BBO 3 REPLACED BY<br>ABU (C11ABU) (NMR, 60<br>STRUCTURES) 1BBO 4 | PROMYELOCYTIC LEUKEMIA<br>ZINC FINGER PROTEIN PLZF; | CHAIN: A;                   |                   |                |                    |                    |               |                              | DNA; CHAIN: A, B, D, E; | CONSENSUS ZINC FINGER    | PROTEIN; CHAIN: C, F, G; |                      |                                         |
| Table 5 | SEQ<br>FOLD     |                                |                                               |                                                           |                                                                                                                                                        |                                                     |                             |                   |                |                    |                    |               |                              |                         |                          |                          |                      |                                         |
| Tal     | PMF             |                                | 0.10                                          |                                                           | 0.15                                                                                                                                                   | 0.95                                                |                             |                   |                |                    |                    |               |                              | 0.22                    |                          |                          |                      |                                         |
|         | Verify<br>score |                                | 0.21                                          |                                                           | -0.11                                                                                                                                                  | 0.25                                                |                             |                   |                |                    |                    |               |                              | -0.36                   |                          |                          |                      |                                         |
|         | Psi<br>Blast    |                                | 3.4e-20                                       |                                                           | 5.1e-05                                                                                                                                                | 1.7e-37                                             |                             |                   |                |                    |                    |               |                              | 6.8e-43                 |                          |                          |                      |                                         |
|         | END<br>AA       |                                | 736                                           |                                                           | 737                                                                                                                                                    | 141                                                 |                             |                   |                |                    |                    |               |                              | 540                     |                          |                          |                      |                                         |
|         | START<br>AA     |                                | 859                                           |                                                           | 889                                                                                                                                                    | 15                                                  |                             |                   |                |                    |                    |               |                              | 461                     |                          |                          |                      |                                         |
|         | CHAIN           |                                | A                                             |                                                           |                                                                                                                                                        | A                                                   |                             |                   |                |                    |                    |               |                              | 3                       |                          |                          |                      |                                         |
|         | PDB<br>ID       |                                | lalh                                          |                                                           | 1bbo                                                                                                                                                   | 1buo                                                |                             |                   |                |                    |                    |               |                              | 1mey                    |                          |                          |                      |                                         |
|         | SEQ<br>ID       |                                | 1856                                          |                                                           | 1856                                                                                                                                                   | 1856                                                |                             |                   |                |                    |                    |               |                              | 1856                    |                          |                          |                      |                                         |

|         | PDB annotation | •     | (ZINC FINGER/DNA) | COMPLEX (ZINC<br>FINGER/DNA) ZINC FINGER,        | PROTEIN-DNA              | DESIGN, 2 CRYSTAL | STRUCTURE, COMPLEX | (CILLO LINOLINA) | COMPLEX (ZINC FINGER, FINGER, DATE OF THE FINGER PROBLEM OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE OF THE O | PROTEIN-DNA              | INTERACTION, PROTEIN | DESIGN, 2 CRYSTAL | STRUCTURE, COMPLEX | (ZINC FINGER/DNA) | COMPLEX (ZINC           | FINGER/DNA) ZINC FINGER, | PROTEIN-DNA              | INTERACTION, PROTEIN | DESIGN, 2 CRYSTAL | STRUCTURE, COMPLEX | (ZINC FINGER/DNA) | COMPLEX (ZINC           | FINGER/DNA) ZINC FINGER, | PROTEIN-DNA              | INTERACTION, PROTEIN | DESIGN, 2 CRYSTAL | STRUCTURE, COMPLEX | (ZINC FINGER/DNA) | COMPLEX (ZINC<br>FINGER/DNA) ZINC FINGER,        |
|---------|----------------|-------|-------------------|--------------------------------------------------|--------------------------|-------------------|--------------------|------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------|----------------------|-------------------|--------------------|-------------------|-------------------------|--------------------------|--------------------------|----------------------|-------------------|--------------------|-------------------|-------------------------|--------------------------|--------------------------|----------------------|-------------------|--------------------|-------------------|--------------------------------------------------|
|         | Compound       |       |                   | DNA; CHAIN: A, B, D, E;<br>CONSENSUS ZINC FINGER | PROTEIN; CHAIN: C, F, G; |                   |                    |                  | DNA; CHAIN: A, B, D, E;<br>CONSENSUS ZINC FINGER                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | PROTEIN; CHAIN: C, F, G; |                      |                   |                    |                   | DNA; CHAIN: A, B, D, E; | CONSENSUS ZINC FINGER    | PROTEIN; CHAIN: C, F, G; |                      |                   |                    |                   | DNA; CHAIN: A, B, D, E; | CONSENSUS ZINC FINGER    | PROTEIN; CHAIN: C, F, G; |                      |                   |                    |                   | DNA; CHAIN: A, B, D, E;<br>CONSENSUS ZINC FINGER |
| Table 5 | SEQ            | score |                   |                                                  |                          |                   |                    |                  |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |                          |                      |                   |                    |                   |                         |                          |                          |                      |                   |                    |                   |                         |                          |                          |                      |                   |                    |                   | 83.92                                            |
| Ta      | PMF            | 7005  |                   | 0.53                                             |                          |                   |                    |                  | 0.99                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |                          |                      |                   |                    |                   | 1.00                    |                          |                          |                      |                   |                    |                   | 1.00                    |                          |                          |                      |                   |                    |                   |                                                  |
|         | Verify         |       |                   | -0.14                                            |                          |                   |                    |                  | 0.23                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |                          |                      |                   |                    |                   | 0.19                    |                          |                          |                      |                   |                    |                   | 0.15                    |                          |                          |                      |                   |                    |                   |                                                  |
|         | Psi<br>Rlast   | Ciasi |                   | 6.8e-48                                          |                          |                   |                    |                  | 1.7e-49                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |                          |                      |                   |                    |                   | 1.5e-49                 |                          |                          |                      |                   |                    |                   | 5.1e-50                 |                          |                          |                      |                   |                    |                   | 3.4e-50                                          |
|         | END<br>A A     | 177   |                   | 869                                              |                          |                   |                    |                  | 626                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |                          |                      |                   |                    |                   | 654                     |                          |                          |                      |                   |                    |                   | 682                     |                          |                          |                      |                   |                    |                   | 710                                              |
|         | START<br>A A   | 42    |                   | 515                                              |                          |                   |                    |                  | 545                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |                          |                      |                   |                    |                   | 573                     |                          |                          |                      |                   |                    |                   | 601                     |                          |                          |                      |                   |                    |                   | 629                                              |
|         | CHAIN          | 3     |                   | C                                                |                          |                   |                    |                  | ن<br>ن                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |                          |                      |                   |                    |                   | 2                       |                          |                          |                      |                   |                    |                   | 3                       |                          |                          |                      |                   |                    |                   | ပ                                                |
|         | PDB            | 3     |                   | 1mey                                             |                          | ,                 |                    |                  | 1mey                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |                          |                      |                   |                    |                   | 1mey                    |                          |                          |                      | -                 |                    |                   | 1mey                    |                          |                          |                      |                   |                    | -                 | 1mey                                             |
|         | SEQ            | <br>9 |                   | 1856                                             |                          |                   |                    |                  | 1856                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |                          | <del></del>          |                   |                    |                   | 1856                    |                          |                          |                      |                   |                    |                   | 1856                    |                          |                          |                      |                   |                    |                   | 1856                                             |

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|         | PDB annotation       | PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC<br>FINGER/DNA) ZINC FINGER,<br>PROTEIN-DNA<br>INTERACTION, PROTEIN<br>DESIGN, 2 CRYSTAL<br>STRUCTURE, COMPLEX<br>(ZINC FINGER/DNA) | COMPLEX (ZINC<br>FINGER/DNA) ZINC FINGER,<br>PROTEIN-DNA<br>INTERACTION, PROTEIN<br>DESIGN, 2 CRYSTAL<br>STRUCTURE, COMPLEX<br>(ZINC FINGER/DNA) | TRANSFERASE ALPHA-<br>SUPERHELIX,<br>TRANSFERASE      | CONTRACTILE PROTEIN TRIPLE-HELIX COILED COIL, CONTRACTILE PROTEIN | ISOMERASE ISOMERASE,<br>MUTASE,<br>INTRAMOLECULAR<br>TRANSFERASE | ISOMERASE ISOMERASE, |
|---------|----------------------|-----------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------|-------------------------------------------------------------------|------------------------------------------------------------------|----------------------|
|         |                      | PROTEIN-DNA INTERACTION DESIGN, 2 CRY STRUCTURE, ( ZINC FINGER                          | COMPLEX (ZIP<br>FINGER/DNA)<br>PROTEIN-DNA<br>INTERACTION<br>DESIGN, 2 CRY<br>STRUCTURE, C                                                       | COMPLEX (ZIN<br>FINGER/DNA).<br>PROTEIN-DNA<br>INTERACTION<br>DESIGN, 2 CRY<br>STRUCTURE, (ZINC FINGER,                                          | TRANSFERAS<br>SUPERHELIX,<br>TRANSFERAS               | CONTRA(<br>TRIPLE-H<br>COIL, COI                                  | ISOMERA<br>MUTASE,<br>INTRAMC<br>TRANSFE                         | ISOMEF               |
|         | Compound             | PROTEIN; CHAIN: C, F, G;                                                                | DNA; CHAIN: A, B, D, E;<br>CONSENSUS ZINC FINGER<br>PROTEIN; CHAIN: C, F, G;                                                                     | DNA; CHAIN: A, B, D, E;<br>CONSENSUS ZINC FINGER<br>PROTEIN; CHAIN: C, F, G;                                                                     | SOLUBLE LYTIC<br>TRANSGLYCOSYLASE SLT70;<br>CHAIN: A; | HUMAN SKELETAL MUSCLE<br>ALPHA-ACTININ 2; CHAIN: A;               | METHYLMALONYL-COA<br>MUTASE; CHAIN: A, B, C, D;                  | METHYLMALONYL-COA    |
| Table 5 | SEQ<br>FOLD<br>score |                                                                                         |                                                                                                                                                  |                                                                                                                                                  |                                                       |                                                                   |                                                                  |                      |
| Tal     | PMF                  |                                                                                         | 1.00                                                                                                                                             | 0.94                                                                                                                                             | -0.20                                                 | -0.20                                                             | -0.20                                                            | -0.20                |
|         | Verify<br>score      |                                                                                         | 0.29                                                                                                                                             | 0.32                                                                                                                                             | 0.27                                                  | 1.02                                                              | 0.15                                                             | 0.73                 |
|         | Psi<br>Blast         |                                                                                         | 3.4e-50                                                                                                                                          | 3.4e-37                                                                                                                                          | 1.8e-08                                               | 4.4e-09                                                           | 4.4e-14                                                          | 6.6e-18              |
|         | END<br>AA            |                                                                                         | 710                                                                                                                                              | 736                                                                                                                                              | 387                                                   | 380                                                               | 379                                                              | 423                  |
|         | START<br>AA          |                                                                                         | 629                                                                                                                                              | 657                                                                                                                                              | 296                                                   | 301                                                               | 218                                                              | 306                  |
|         | CHAIN                |                                                                                         | U                                                                                                                                                | O                                                                                                                                                | A                                                     | V V                                                               | А                                                                | А                    |
|         | PDB<br>ID            |                                                                                         | 1mey                                                                                                                                             | Imey                                                                                                                                             | 1qsa                                                  | 1quu                                                              | lreq                                                             | 1req                 |
|         | SEQ<br>ID<br>NO:     |                                                                                         | 1856                                                                                                                                             | 1856                                                                                                                                             | 1856                                                  | 1856                                                              | 1856                                                             | 1856                 |

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|---------|----------------------|------------------------------------------|----------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------|
|         | PDB annotation       | MUTASE,<br>INTRAMOLECULAR<br>TRANSFERASE | ZINC FINGER TRANSCRIPTION FACTOR SP1; ZINC FINGER, TRANSCRIPTION ACTIVATION, SP1 | COMPLEX (TRANSCRIPTION<br>REGULATION/DNA) TFIIIA;<br>5S GENE; NMR, TFIIIA,<br>PROTEIN, DNA,<br>TRANSCRIPTION FACTOR,<br>5S RNA 2 GENE, DNA<br>BINDING PROTEIN, ZINC<br>FINGER, COMPLEX 3<br>(TRANSCRIPTION<br>REGULATION/DNA) | COMPLEX (TRANSCRIPTION<br>REGULATION/DNA) TFIIIA;<br>5S GENE; NMR, TFIIIA,<br>PROTEIN, DNA,<br>TRANSCRIPTION FACTOR,<br>5S RNA 2 GENE, DNA<br>BINDING PROTEIN, ZINC<br>FINGER, COMPLEX 3<br>(TRANSCRIPTION<br>REGULATION/DNA) | COMPLEX (TRANSCRIPTION REGULATION/DNA) COMPLEX (TRANSCRIPTION        |
|         | Compound             | MUTASE; CHAIN: A, B, C, D;               | SP1F2; CHAIN: NULL;                                                              | TRANSCRIPTION FACTOR IIIA;<br>CHAIN: A; 5S RNA GENE;<br>CHAIN: E, F;                                                                                                                                                          | TRANSCRIPTION FACTOR IIIA;<br>CHAIN: A; 5S RNA GENE;<br>CHAIN: E, F;                                                                                                                                                          | TFIIIA; CHAIN: A, D; 5S<br>RIBOSOMAL RNA GENE; CHAIN:<br>B, C, E, F; |
| Table 5 | SEQ<br>FOLD<br>score |                                          |                                                                                  |                                                                                                                                                                                                                               |                                                                                                                                                                                                                               |                                                                      |
| Tal     | PMF                  |                                          | 0.37                                                                             | 0.05                                                                                                                                                                                                                          | 0.59                                                                                                                                                                                                                          | 0.31                                                                 |
|         | Verify<br>score      |                                          | -0.25                                                                            | 0.01                                                                                                                                                                                                                          | -0.22                                                                                                                                                                                                                         | -0.41                                                                |
|         | Psi<br>Blast         |                                          | 6.8e-06                                                                          | 8.5e-17                                                                                                                                                                                                                       | 3.4e-21                                                                                                                                                                                                                       | 5.1e-34                                                              |
|         | END                  |                                          | 714                                                                              | 540                                                                                                                                                                                                                           | 626                                                                                                                                                                                                                           | 614                                                                  |
|         | START                |                                          | 989                                                                              | 462                                                                                                                                                                                                                           | 546                                                                                                                                                                                                                           | 462                                                                  |
|         | CHAIN                | -                                        |                                                                                  | A                                                                                                                                                                                                                             | A                                                                                                                                                                                                                             | A                                                                    |
|         | PDB                  |                                          | 1sp2                                                                             | 143                                                                                                                                                                                                                           | 145                                                                                                                                                                                                                           | 14f6                                                                 |
|         | SEQ<br>NO:           |                                          | 1856                                                                             | 1856                                                                                                                                                                                                                          | 1856                                                                                                                                                                                                                          | 1856                                                                 |

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| PDB annotatic | Compound | SEO     | PMF | Verify | Psi | END | START | CHAIN |
|               |          | ole 5   | La  |        |     |     |       |       |
|               |          | Table 5 | Ta  |        |     |     |       |       |

|         |                      |                                                            |                                    |                         |                                           |                      |                                    |                         |         |                                                       |                        |                      |                   |               |                                    | т—                      |                            |                        |                       |                   |                 |                         |                         |                            |
|---------|----------------------|------------------------------------------------------------|------------------------------------|-------------------------|-------------------------------------------|----------------------|------------------------------------|-------------------------|---------|-------------------------------------------------------|------------------------|----------------------|-------------------|---------------|------------------------------------|-------------------------|----------------------------|------------------------|-----------------------|-------------------|-----------------|-------------------------|-------------------------|----------------------------|
|         | PDB annotation       | REGULATION/DNA), RNA<br>POLYMERASE III, 2<br>TRANSCRIPTION | INITIATION, ZINC FINGER<br>PROTEIN | COMPLEX (TRANSCRIPTION  | KEGULATION/DNA)<br>COMPLEX (TRANSCRIPTION | REGULATION/DNA), RNA | FOLTMERASE III, 2<br>TRANSCRIPTION | INITIATION, ZINC FINGER | PROTEIN | COMPLEX (TRANSCRIPTION REGIT ATTON/DNA)               | COMPLEX (TRANSCRIPTION | REGULATION/DNA), RNA | POLYMERASE III, 2 | IKANSCKIPIJON | INITIATION, ZINC FINGER<br>PROTEIN | COMPLEX (TRANSCRIPTION  | REGULATION/DNA)            | COMPLEX (TRANSCRIPTION | KEGULA HUN/DINA), KNA | POLYMERASE III, 2 | I KANSCKIF HOIN | INITIATION, ZINC FINGER | COMPLEX (TRANSCRIPTION  | REGULATION/DNA)            |
|         | Compound             | -                                                          |                                    | TFIIIA; CHAIN: A, D; 5S | KIBOSOMAL KNA GENE; CHAIN:<br>B, C, E, F; |                      |                                    |                         |         | TFIIIA; CHAIN: A, D; 5S<br>RIBOSOMAI RNA GENF: CHAIN: | B, C, E, F;            |                      |                   |               |                                    | TFIIIA; CHAIN: A, D; 5S | RIBOSOMAL RNA GENE; CHAIN: | B, C, E, F;            |                       |                   |                 |                         | TFIIIA; CHAIN: A, D; 5S | RIBOSOMAL RNÁ GENE; CHAIN: |
| Table 5 | SEQ<br>FOLD<br>score |                                                            |                                    |                         |                                           |                      |                                    |                         |         | 98.94                                                 |                        |                      |                   |               |                                    |                         |                            |                        |                       |                   |                 |                         |                         |                            |
| Tar     | PMF                  |                                                            |                                    | 0.15                    |                                           | , , , , ,            |                                    |                         |         |                                                       |                        |                      |                   |               |                                    | 96.0                    |                            |                        |                       |                   |                 |                         | 96.0                    | }                          |
|         | Verify<br>score      |                                                            |                                    | -0.23                   |                                           |                      |                                    |                         |         |                                                       |                        |                      |                   |               |                                    | -0.12                   |                            |                        |                       |                   |                 |                         | -0.07                   |                            |
|         | Psi<br>Blast         |                                                            |                                    | 6.8e-37                 |                                           |                      |                                    |                         |         | 2.2e-44                                               |                        |                      |                   |               |                                    | 1.7e-38                 |                            |                        |                       |                   |                 |                         | 2.2e-44                 |                            |
|         | END                  |                                                            |                                    | 663                     |                                           |                      |                                    |                         |         | 711                                                   |                        |                      |                   |               |                                    | 691                     |                            |                        |                       |                   |                 |                         | 707                     |                            |
|         | START<br>AA          |                                                            |                                    | 516                     |                                           |                      |                                    |                         |         | 545                                                   |                        |                      |                   |               |                                    | 546                     |                            |                        |                       |                   |                 |                         | 546                     | 2                          |
|         | CHAIN<br>ID          |                                                            |                                    | A                       |                                           |                      |                                    |                         |         | A                                                     |                        |                      |                   |               |                                    | A                       |                            |                        |                       |                   |                 |                         | A                       | 1                          |
|         | PDB<br>ID            |                                                            |                                    | 1tf6                    |                                           |                      |                                    |                         |         | 1tf6                                                  |                        |                      |                   |               |                                    | 1tf6                    |                            |                        |                       |                   |                 |                         | 1116                    | OT:                        |
|         | SEQ<br>D<br>NO:      |                                                            |                                    | 1856                    |                                           |                      |                                    |                         |         | 1856                                                  |                        |                      |                   |               |                                    | 1856                    |                            |                        |                       |                   | _               |                         | 1856                    |                            |
|         |                      |                                                            |                                    |                         |                                           |                      |                                    |                         |         |                                                       |                        |                      |                   |               |                                    |                         |                            |                        |                       |                   |                 |                         |                         |                            |

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|         | PDB annotation       | COMPLEX (TRANSCRIPTION<br>REGULATION/DNA), RNA<br>POLYMERASE III, 2<br>TRANSCRIPTION<br>INITIATION, ZINC FINGER<br>PROTEIN | COMPLEX (TRANSCRIPTION REGULATION/DNA) COMPLEX (TRANSCRIPTION REGULATION/DNA), RNA POLYMERASE III, 2 TRANSCRIPTION INITIATION, ZINC FINGER PROTEIN | COMPLEX (TRANSCRIPTION<br>REGULATION/DNA)<br>COMPLEX (TRANSCRIPTION<br>REGULATION/DNA), RNA<br>POLYMERASE III, 2<br>TRANSCRIPTION<br>INITIATION, ZINC FINGER<br>PROTEIN | COMPLEX (TRANSCRIPTION REGULATION/DNA) YING-YANG 1; TRANSCRIPTION INITIATOR ELEMENT, YY1, ZINC 2 FINGER PROTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULATION/DNA) |
|---------|----------------------|----------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
|         | Compound             | B, C, B, F;                                                                                                                | TFIIIA; CHAIN: A, D; 5S<br>RIBOSOMAL RNA GENE; CHAIN:<br>B, C, E, F;                                                                               | TFIIIA; CHAIN: A, D; 5S<br>RIBOSOMAL RNA GENE; CHAIN:<br>B, C, E, F;                                                                                                    | YY1; CHAIN: C; ADENO-<br>ASSOCIATED VIRUS P5<br>INITIATOR ELEMENT DNA;<br>CHAIN: A, B;                                                                                             |
| Table 5 | SEQ<br>FOLD<br>score |                                                                                                                            |                                                                                                                                                    |                                                                                                                                                                         |                                                                                                                                                                                    |
| I al    | PMF                  |                                                                                                                            | 0.99                                                                                                                                               | 0.54                                                                                                                                                                    | 0.04                                                                                                                                                                               |
|         | Verify<br>score      |                                                                                                                            | 0.22                                                                                                                                               | 0.20                                                                                                                                                                    | -0.73                                                                                                                                                                              |
|         | Psi<br>Blast         |                                                                                                                            | 1.5e-38                                                                                                                                            | 3.4e-30                                                                                                                                                                 | 6.8e-27                                                                                                                                                                            |
|         | END                  |                                                                                                                            | 716                                                                                                                                                | 737                                                                                                                                                                     | 540                                                                                                                                                                                |
|         | START<br>AA          |                                                                                                                            | 575                                                                                                                                                | 602                                                                                                                                                                     | 442                                                                                                                                                                                |
|         | CHAIN<br>ID          |                                                                                                                            | ∢                                                                                                                                                  | ¥                                                                                                                                                                       | U                                                                                                                                                                                  |
|         | PDB<br>ID            |                                                                                                                            | 1476                                                                                                                                               | 1116                                                                                                                                                                    | lubd                                                                                                                                                                               |
|         | SEQ<br>ED SEQ        |                                                                                                                            | 1856                                                                                                                                               | 1856                                                                                                                                                                    | 1856                                                                                                                                                                               |

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|---------|----------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------|
|         | PDB annotation       | COMPLEX (TRANSCRIPTION<br>REGULATION/DNA) YING-<br>YANG 1; TRANSCRIPTION<br>INITIATION, INITIATOR<br>ELEMENT, YY1, ZINC 2<br>FINGER PROTEIN, DNA-<br>PROTEIN RECOGNITION, 3<br>COMPLEX (TRANSCRIPTION<br>REGULATION/DNA) | COMPLEX (TRANSCRIPTION REGULATION/DNA) YING-YANG 1; TRANSCRIPTION INITIATOR ELEMENT, YY1, ZINC 2 FINGER PROTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULATION/DNA) | COMPLEX (TRANSCRIPTION REGULATION/DNA) YING-YANG 1; TRANSCRIPTION INITIATION INITIATOR ELEMENT, YY1, ZINC 2 FINGER PROTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULATION/DNA) | COMPLEX (TRANSCRIPTION REGULATION/DNA) YING-YANG 1; TRANSCRIPTION INITIATION           |
|         | Compound             | YY1; CHAIN: C; ADENO-<br>ASSOCIATED VIRUS P5<br>INITIATOR ELEMENT DNA;<br>CHAIN: A, B;                                                                                                                                   | YY1; CHAIN: C; ADENO-<br>ASSOCIATED VIRUS P5<br>INITIATOR ELEMENT DNA;<br>CHAIN: A, B;                                                                                             | YY1; CHAIN: C; ADENO-<br>ASSOCIATED VIRUS P5<br>INITIATOR ELEMENT DNA;<br>CHAIN: A, B;                                                                                                        | YY1; CHAIN: C; ADENO-<br>ASSOCIATED VIRUS P5<br>INITIATOR ELEMENT DNA;<br>CHAIN: A, B; |
| Table 5 | SEQ<br>FOLD<br>score |                                                                                                                                                                                                                          |                                                                                                                                                                                    |                                                                                                                                                                                               | 78.17                                                                                  |
| Tal     | PMF                  | 0.01                                                                                                                                                                                                                     | 0.25                                                                                                                                                                               | 0.55                                                                                                                                                                                          |                                                                                        |
|         | Verify<br>score      | -0.62                                                                                                                                                                                                                    | -0.36                                                                                                                                                                              | -0.35                                                                                                                                                                                         |                                                                                        |
|         | Psi<br>Blast         | 3.4e-30                                                                                                                                                                                                                  | 8.8e-24                                                                                                                                                                            | 1e-33                                                                                                                                                                                         | 5.1e-35                                                                                |
|         | END                  | 570                                                                                                                                                                                                                      | 626                                                                                                                                                                                | 598                                                                                                                                                                                           | 655                                                                                    |
|         | START<br>AA          | 469                                                                                                                                                                                                                      | 493                                                                                                                                                                                | 496                                                                                                                                                                                           | 547                                                                                    |
|         | CHAIN                | U                                                                                                                                                                                                                        | U                                                                                                                                                                                  | U                                                                                                                                                                                             | O                                                                                      |
|         | PDB<br>ID            | lubd                                                                                                                                                                                                                     | lubd                                                                                                                                                                               | lubd                                                                                                                                                                                          | 1ubd                                                                                   |
|         | SEQ<br>ID<br>NO:     | 1856                                                                                                                                                                                                                     | 1856                                                                                                                                                                               | 1856                                                                                                                                                                                          | 1856                                                                                   |

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| np        | FDB annotation   |             | ELEMENT, YY1, ZINC 2<br>FINGER PROTEIN, DNA- | COMPLEX (TRANSCRIPTION | REGULATION/DNA) | COMPLEX (TRANSCRIPTION | REGULATION/DNA) YING- | YANG 1; TRANSCRIPTION<br>INITIATION, INITIATOR | ELEMENT, YY1, ZINC 2 | FINGER PROTEIN, DNA- | PROTEIN RECOGNITION, 3 | COMPLEX (TRANSCRIPTION | REGULATION/DNA) | COMPLEX (TRANSCRIPTION | REGULATION/DNA) YING- | YANG 1; TRANSCRIPTION  | INITIATION, INITIATOR | ELEMENT, YY1, ZINC 2 | FINGER PROTEIN, DNA- | PROTEIN RECOGNITION, 3 | COMPLEX (TRANSCRIPTION | REGULATION/DNA) | COMPLEX (TRANSCRIPTION | REGULATION/DNA) YING- | YANG 1; TRANSCRIPTION  | INITIATION, INITIATOR | ELEMENT, YY1, ZINC 2 | FINGER PROTEIN, DNA- | PROTEIN RECOGNITION, 3<br>COMPLEX (TRANSCRIPTION |
|-----------|------------------|-------------|----------------------------------------------|------------------------|-----------------|------------------------|-----------------------|------------------------------------------------|----------------------|----------------------|------------------------|------------------------|-----------------|------------------------|-----------------------|------------------------|-----------------------|----------------------|----------------------|------------------------|------------------------|-----------------|------------------------|-----------------------|------------------------|-----------------------|----------------------|----------------------|--------------------------------------------------|
|           | Compound         |             |                                              |                        |                 | YY1; CHAIN: C; ADENO-  | ASSOCIATED VIRUS P5   | INITIATOR ELEMENT DNA;<br>CHAIN: A. B:         |                      |                      |                        |                        |                 | YY1; CHAIN: C; ADENO-  | ASSOCIATED VIRUS P5   | INITIATOR ELEMENT DNA; | CHAIN: A, B;          |                      |                      |                        |                        |                 | YY1; CHAIN: C; ADENO-  | ASSOCIATED VIRUS P5   | INITIATOR ELEMENT DNA; | CHAIN: A, B;          |                      |                      |                                                  |
| Table 3   | FOLD             | score       |                                              |                        |                 |                        |                       |                                                |                      |                      |                        |                        |                 |                        |                       |                        |                       |                      |                      |                        |                        |                 |                        |                       |                        |                       |                      |                      |                                                  |
| I at      | FIMIF            |             |                                              |                        |                 | 0.40                   |                       |                                                |                      |                      |                        |                        |                 | 96.0                   |                       |                        |                       |                      |                      |                        |                        |                 | 1.00                   |                       | •                      |                       |                      |                      |                                                  |
| J. 11     | v errry<br>score |             |                                              |                        |                 | -0.30                  |                       |                                                |                      |                      |                        |                        |                 | 0.11                   |                       |                        |                       |                      |                      |                        |                        |                 | -0.12                  |                       |                        |                       |                      |                      |                                                  |
|           | FSI<br>Blast     |             |                                              |                        |                 | 4.4e-31                |                       |                                                |                      |                      |                        |                        |                 | 5.1e-35                |                       |                        |                       | •                    |                      |                        |                        |                 | 5.1e-35                |                       |                        |                       |                      |                      |                                                  |
| 4         | END<br>AA        |             |                                              |                        |                 | 682                    |                       |                                                |                      |                      |                        |                        |                 | 654                    |                       |                        |                       |                      |                      |                        |                        |                 | 710                    |                       |                        |                       |                      |                      |                                                  |
| T-C-4-T-C | SIAKI            | i<br>I      |                                              |                        |                 | 550                    | •                     |                                                |                      | -                    |                        |                        |                 | 553                    |                       |                        |                       |                      |                      |                        |                        |                 | 609                    |                       |                        |                       |                      |                      |                                                  |
| THEFT     | CHAIN            | ١.          |                                              |                        |                 | 2                      |                       |                                                |                      |                      |                        |                        |                 | 2                      |                       |                        |                       |                      |                      |                        |                        |                 | ၁                      |                       |                        |                       |                      | . —                  |                                                  |
| ממת       | FDB<br>ID        | <u> </u>    |                                              |                        |                 | 1ubd                   |                       |                                                |                      |                      |                        |                        |                 | 1ubd                   |                       |                        |                       |                      |                      |                        |                        |                 | 1ubd                   |                       |                        |                       |                      |                      |                                                  |
| CES       | )<br>H           | i<br>S<br>N |                                              |                        |                 | 1856                   |                       |                                                |                      |                      |                        |                        |                 | 1856                   |                       |                        |                       |                      |                      |                        |                        |                 | 1856                   |                       |                        |                       |                      |                      |                                                  |

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|---------|----------------|-------|-----------------|----------------------------------------------|------------------------|-----------------------|----------------------|----------------------|------------------------|------------------------|-----------------|------------------------|-----------------------|------------------------|-----------------------|----------------------|----------------------|------------------------|------------------------|-----------------|--------------------|------------|---------------|------------------------|-------------|---------------------------|-----------------------------|-----------------------|-----------------------|----------------------|----------------------------------------------------------|
|         | PDB annotation |       | REGULATION/DNA) | COMPLEX (TRANSCRIPTION REGULATION/DNA) YING- | YANG 1; TRANSCRIPTION  | INITIATION, INITIATOR | ELEMENT, YY1, ZINC 2 | FINGER PROTEIN, DNA- | PROTEIN RECOGNITION, 3 | COMPLEX (TRANSCRIPTION | REGULATION/DNA) | COMPLEX (TRANSCRIPTION | REGULATION/DNA) YING- | YANG 1; TRANSCRIPTION  | INITIATION, INITIATOR | ELEMENT, YY1, ZINC 2 | FINGER PROTEIN, DNA- | PROTEIN RECOGNITION, 3 | COMPLEX (TRANSCRIPTION | REGULATION/DNA) | TRANSCRIPTION      | REGULATION | TRANSCRIPTION | REGULATION, ADR1, ZINC | FINGER, NMR | COMPLEX (DNA-BINDING      | PROTEIN/DNA) FIVE-          | FINGER GLI; GLI, ZINC | FINGER, COMPLEX (DNA- | BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE-                  |
|         | Compound       |       | -               | YY1; CHAIN: C; ADENO-<br>ASSOCIATED VIRUS P5 | INITIATOR ELEMENT DNA; | CHAIN: A, B;          |                      |                      |                        |                        |                 | YY1; CHAIN: C; ADENO-  | ASSOCIATED VIRUS P5   | INITIATOR ELEMENT DNA; | CHAIN: A, B;          |                      |                      |                        |                        |                 | ADR1; CHAIN: NULL; |            |               |                        |             | ZINC FINGER PROTEIN GLI1; | CHAIN: A; DNA; CHAIN: C, D; |                       |                       |                      | ZINC FINGER PROTEIN GLII;<br>CHAIN: A; DNA; CHAIN: C, D; |
| Table 5 | SEQ            | roll  |                 |                                              |                        |                       |                      |                      |                        |                        |                 |                        |                       |                        |                       |                      |                      |                        |                        |                 |                    |            |               |                        |             |                           |                             |                       |                       |                      |                                                          |
| Tab     | PMF            | score |                 | 0.94                                         |                        |                       |                      |                      |                        |                        |                 | 0.29                   |                       |                        |                       |                      |                      |                        |                        |                 | 0.94               |            |               |                        |             | 0.37                      |                             |                       |                       |                      | 0.41                                                     |
|         | Verify         | score |                 | 0.12                                         |                        |                       |                      |                      |                        |                        |                 | -0.13                  |                       |                        |                       |                      |                      |                        |                        |                 | -0.04              |            |               |                        |             | -0.40                     |                             |                       |                       |                      | -0.18                                                    |
|         | Psi            | Blast |                 | 1.7e-25                                      |                        |                       |                      |                      |                        |                        |                 | 1.2e-13                |                       |                        |                       |                      |                      |                        |                        |                 | 1.1e-19            |            |               |                        |             | 1.7e-26                   |                             |                       |                       |                      | 3.4e-33                                                  |
|         | END            | AA    |                 | 731                                          |                        |                       |                      |                      |                        |                        |                 | 736                    |                       |                        |                       |                      |                      |                        |                        |                 | 716                |            |               |                        |             | 569                       |                             |                       |                       |                      | 625                                                      |
|         | START          | AA    | *               | 637                                          |                        |                       |                      |                      |                        |                        |                 | 999                    |                       |                        |                       |                      |                      |                        |                        |                 | 859                |            |               |                        |             | 441                       |                             |                       |                       |                      | 496                                                      |
|         | CHAIN          | 3     |                 | O                                            |                        |                       |                      |                      |                        |                        |                 | C                      |                       |                        |                       |                      |                      |                        |                        |                 |                    |            |               |                        |             | A                         |                             |                       |                       |                      | A                                                        |
|         | PDB            | a     |                 | 1ubd                                         |                        |                       |                      |                      |                        |                        |                 | 1ubd                   | -                     |                        |                       |                      |                      |                        |                        |                 | 2adr               |            |               |                        |             | 2gli                      | _                           |                       |                       |                      | 2gli                                                     |
|         | SEQ            | a ÿ   |                 | 1856                                         |                        |                       |                      |                      |                        |                        |                 | 1856                   |                       |                        |                       |                      |                      |                        |                        |                 | 1856               |            |               |                        |             | 1856                      |                             |                       |                       |                      | 1856                                                     |

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|         | PDB annotation |       | FINGER GLI; GLI, ZINC<br>FINGER, COMPLEX (DNA-<br>BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING      | PROTEIN/DNA) FIVE-<br>FINGER GLI; GLI, ZINC | FINGER, COMPLEX (DNA- | BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING      | FROI EIN/DINA) FIVE-        | FINGER COMPLEX (DNA- | BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING      | PROTEIN/DNA) FIVE-          | FINGER GLI; GLI, ZINC | FINGER, COMPLEX (DNA- | BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING      | PROTEIN/DNA) FIVE-          | FINGER GLI; GLI, ZINC | FINGER, COMPLEX (DNA- | BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING      | PROTEIN/DNA) FIVE-          | FINGER GLI; GLI, ZINC | FINGER, COMPLEX (DNA- | BINDING PROTEIN/DNA) |                         |                            |
|---------|----------------|-------|------------------------------------------------------------------------|---------------------------|---------------------------------------------|-----------------------|----------------------|---------------------------|-----------------------------|----------------------|----------------------|---------------------------|-----------------------------|-----------------------|-----------------------|----------------------|---------------------------|-----------------------------|-----------------------|-----------------------|----------------------|---------------------------|-----------------------------|-----------------------|-----------------------|----------------------|-------------------------|----------------------------|
|         | Compound       |       |                                                                        | ZINC FINGER PROTEIN GLII; | CHAIN: A; DNA; CHAIN: C, D;                 |                       |                      | ZINC FINGER PROTEIN GL11; | CHAIN: A; DNA; CHAIN: C, D; |                      |                      | ZINC FINGER PROTEIN GLII; | CHAIN: A; DNA; CHAIN: C, D; |                       |                       |                      | ZINC FINGER PROTEIN GLII; | CHAIN: A; DNA; CHAIN: C, D; |                       |                       |                      | ZINC FINGER PROTEIN GLI1; | CHAIN: A; DNA; CHAIN: C, D; |                       |                       |                      | ZINC FINGER DNA BINDING | SWAP) (NMR, 12 STRUCTURES) |
| Table 5 | SEQ            | FOLD  |                                                                        |                           |                                             |                       |                      | 85.38                     |                             |                      |                      |                           | -                           | - · · -               |                       |                      |                           |                             |                       |                       |                      |                           |                             |                       |                       |                      |                         |                            |
| Tat     | PMF            | score |                                                                        | 0.84                      |                                             |                       |                      |                           |                             |                      |                      | 96.0                      |                             |                       |                       |                      | 89.0                      |                             |                       |                       |                      | 69.0                      |                             |                       |                       |                      | 0.53                    |                            |
|         | Verify         | score |                                                                        | -0.07                     |                                             |                       |                      |                           |                             |                      |                      | 0.33                      |                             |                       |                       |                      | 0.12                      |                             |                       |                       |                      | 0.14                      |                             |                       |                       |                      | -0.19                   |                            |
|         | Psi            | Blast |                                                                        | 8.8e-42                   |                                             |                       |                      | 4.4e-42                   |                             |                      |                      | 4.4e-42                   |                             |                       |                       |                      | 1.2e-34                   |                             |                       |                       |                      | 1.7e-27                   |                             |                       |                       |                      | 0.00012                 |                            |
|         | END            | AA    |                                                                        | 684                       |                                             |                       |                      | 712                       |                             |                      |                      | 707                       |                             |                       |                       |                      | 709                       |                             |                       |                       |                      | 736                       |                             |                       |                       |                      | 714                     |                            |
|         | START          | AA    |                                                                        | 545                       |                                             |                       |                      | 573                       |                             |                      |                      | 575                       |                             |                       |                       |                      | 581                       |                             |                       |                       |                      | 609                       |                             |                       |                       |                      | 989                     |                            |
|         | CHAIN          | О     |                                                                        | A                         |                                             |                       |                      | A                         |                             |                      |                      | A                         |                             |                       |                       |                      | A                         |                             |                       |                       |                      | A                         |                             |                       |                       |                      |                         |                            |
|         | PDB            | A     |                                                                        | 2gli                      |                                             |                       |                      | 2gli                      |                             |                      | •                    | 20li                      | 50                          |                       |                       |                      | 2gli                      | )                           |                       |                       |                      | 2gli                      | )                           |                       |                       |                      | 7znf                    |                            |
|         | SEQ            | A Ş   |                                                                        | 1856                      |                                             |                       |                      | 1856                      |                             |                      |                      | 1856                      |                             |                       |                       |                      | 1856                      |                             |                       |                       |                      | 1856                      |                             |                       |                       |                      | 1856                    |                            |

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Table 5

| PDB annotation |                  |        | COMPLEX                   | (INHIBITOR/NUCLEASE)     | COMPLEX      | (INHIBITOR/NUCLEASE), | COMPLEX (RI-ANG), | RECOGNITION. EPITOPE | MAPPING, LEUCINE-RICH 3 | REPEATS | COMPLEX                 | (INHIBITOR/NUCLEASE)     | COMPLEX      | (INHIBITOR/NUCLEASE), | COMPLEX (KI-ANG), | HYDROLASE 2 MOLECULAR | RECOGNITION, EPITOPE | MAPPING, LEUCINE-RICH 3 | REPEATS | COMPLEX                 | (INHIBITOR/NUCLEASE)     | COMPLEX      | (INHIBITOR/NUCLEASE), | COMPLEX (RI-ANG), | HYDROLASE 2 MOLECULAR | RECOGNITION, EPITOPE | MAPPING, LEUCINE-RICH 3 | REPEATS | COMPLEX (NUCLEAR<br>PROTEIN/RNA) COMPLEX                   |
|----------------|------------------|--------|---------------------------|--------------------------|--------------|-----------------------|-------------------|----------------------|-------------------------|---------|-------------------------|--------------------------|--------------|-----------------------|-------------------|-----------------------|----------------------|-------------------------|---------|-------------------------|--------------------------|--------------|-----------------------|-------------------|-----------------------|----------------------|-------------------------|---------|------------------------------------------------------------|
| Compound       |                  | 7ZNF 3 | RIBONIICI FASE INHIBITOR: | CHAIN: A. D. ANGIOGENIN: | CHAIN: B, E; |                       |                   |                      |                         |         | RIBONUCLEASE INHIBITOR; | CHAIN: A, D; ANGIOGENIN; | CHAIN: B, E; |                       |                   |                       |                      |                         |         | RIBONUCLEASE INHIBITOR; | CHAIN: A, D; ANGIOGENIN; | CHAIN: B, E; |                       |                   |                       |                      |                         |         | U2 RNA HAIRPIN IV; CHAIN: Q, R; U2 A'; CHAIN: A, C; U2 B"; |
| SEO            | FOLD             |        |                           |                          |              |                       |                   |                      |                         |         | 155.44                  |                          | •            |                       |                   |                       |                      |                         |         |                         |                          |              |                       |                   |                       |                      |                         |         |                                                            |
| PMF            | score            |        | 0.17                      | 71.0                     |              |                       |                   |                      |                         |         |                         |                          |              |                       |                   |                       |                      |                         |         | 1.00                    |                          |              |                       |                   |                       |                      |                         |         | 0.09                                                       |
| Verify         | score            |        | 0.04                      | <b>+</b>                 |              |                       |                   |                      |                         |         |                         |                          |              |                       |                   |                       |                      |                         |         | 0.31                    |                          |              |                       |                   |                       |                      |                         |         | -0.44                                                      |
| Psi            | Blast            |        | 15027                     | 13-20-1                  |              | •                     | -                 |                      |                         |         | 3.4e-47                 |                          |              |                       |                   |                       |                      |                         |         | 3.4e-47                 |                          |              |                       |                   |                       |                      |                         |         | 6.8e-05                                                    |
| END            | AA               |        | 170                       | ```                      |              |                       |                   |                      |                         |         | 591                     |                          |              |                       |                   |                       |                      |                         |         | 290                     |                          |              |                       |                   |                       |                      |                         |         | 366                                                        |
| START          | AA               |        | 100                       | 201                      |              |                       |                   |                      |                         |         | 160                     |                          |              |                       | ***               |                       |                      |                         |         | 201                     |                          |              |                       |                   |                       |                      |                         |         | 289                                                        |
| CHAIN          | A<br>A           |        | ***                       | ۲                        |              |                       |                   |                      |                         |         | A                       |                          |              |                       |                   |                       |                      |                         |         | A                       |                          |              |                       |                   | -                     | ,                    |                         |         | А                                                          |
| PINR           |                  |        |                           | 1449                     |              |                       |                   |                      |                         |         | la4y                    | `                        |              |                       | _                 |                       |                      |                         |         | 1a4y                    |                          |              |                       |                   |                       |                      |                         |         | 1a9n                                                       |
| CEO            | A<br>A<br>B<br>B |        | 1071                      | 10/1                     |              |                       |                   |                      |                         |         | 1871                    |                          |              |                       |                   |                       |                      |                         |         | 1871                    |                          |              |                       |                   |                       |                      |                         |         | 1871                                                       |

|         | PDB amotation        | (NUCLEAR PROTEIN/RNA),<br>RNA,<br>SNRNP,RIBONUCLEOPROTE | COMPLEX (NUCLEAR PROTEIN/RNA) COMPLEX (NUCLEAR PROTEIN/RNA), RNA, SNRNP,RIBONUCLEOPROTE | COMPLEX (NUCLEAR PROTEIN/RNA) COMPLEX (NUCLEAR PROTEIN/RNA), RNA, SNRNP, RIBONUCLEOPROTE | COMPLEX (NUCLEAR PROTEIN/RNA) COMPLEX (NUCLEAR PROTEIN/RNA), RNA, SNRNA, SNRNP, RIBONUCLEOPROTE | CELL ADHESION LEUCINE<br>RICH REPEAT, CALCIUM<br>BINDING, CELL ADHESION | CELL ADHESION LEUCINE<br>RICH REPEAT, CALCIUM<br>BINDING, CELL ADHESION | CONTRACTILE PROTEIN<br>LEUCINE-RICH REPEAT,<br>BETA-BETA-ALPHA |
|---------|----------------------|---------------------------------------------------------|-----------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------|-------------------------------------------------------------------------|----------------------------------------------------------------|
|         | Compound             | CHAIN: B, D;                                            | U2 RNA HAIRPIN IV; CHAIN: Q,<br>R; U2 A'; CHAIN: A, C; U2 B";<br>CHAIN: B, D;           | U2 RNA HAIRPIN IV; CHAIN: Q,<br>R; U2 A'; CHAIN: A, C; U2 B";<br>CHAIN: B, D;            | U2 RNA HAIRPIN IV; CHAIN: Q,<br>R; U2 A'; CHAIN: A, C; U2 B";<br>CHAIN: B, D;                   | INTERNALIN B; CHAIN: A;                                                 | INTERNALIN B; CHAIN: A;                                                 | OUTER ARM DYNEIN; CHAIN: A;                                    |
| Table 5 | SEQ<br>FOLD<br>score |                                                         |                                                                                         |                                                                                          |                                                                                                 |                                                                         |                                                                         |                                                                |
| Ta      | PMF                  |                                                         | 0.16                                                                                    | 0.18                                                                                     | 0.54                                                                                            | 0.11                                                                    | 0.00                                                                    | 0.00                                                           |
|         | Verify               |                                                         | 0.37                                                                                    | -0.09                                                                                    | -0.10                                                                                           | -0.42                                                                   | -0.41                                                                   | -0.06                                                          |
|         | Psi<br>Blast         |                                                         | 1e-06                                                                                   | 6e-05                                                                                    | 0.00012                                                                                         | 6.8e-17                                                                 | 0.0048                                                                  | 1e-09                                                          |
|         | END                  |                                                         | 458                                                                                     | 570                                                                                      | 570                                                                                             | 585                                                                     | 589                                                                     | 449                                                            |
|         | START                |                                                         | 360                                                                                     | 454                                                                                      | 454                                                                                             | 383                                                                     | 550                                                                     | 307                                                            |
|         | CHAIN                |                                                         | A                                                                                       | <                                                                                        | U                                                                                               | A                                                                       | A                                                                       | А                                                              |
| 444     | FDB                  |                                                         | 1a9n                                                                                    | 1a9n                                                                                     | 1a9n                                                                                            | 1d0b                                                                    | 1d0b                                                                    | 1ds9                                                           |
| CHO     | A A S                |                                                         | 1871                                                                                    | 1871                                                                                     | 1871                                                                                            | 1871                                                                    | 1871                                                                    | 1871                                                           |

|         | PDB annotation       | CYLINDER, DYNEIN, 2<br>CHLAMYDOMONAS,<br>FLAGELLA | RNA BINDING PROTEIN TAP<br>(NFX1);<br>RIBONUCLEOPROTEIN<br>(RNP,RBD OR RRM) AND<br>LEUCINE-RICH-REPEAT 2<br>(LRR) | RNA BINDING PROTEIN TAP (NFX1); RIBONUCLEOPROTEIN (RNP,RBD OR RRM) AND LEUCINE-RICH-REPEAT 2 (LRR) | RNA BINDING PROTEIN TAP (NFX1); RIBONUCLEOPROTEIN (RNP,RBD OR RRM) AND LEUCINE-RICH-REPEAT 2 (LRR) | LIGASE CYCLIN A/CDK2-<br>ASSOCIATED PROTEIN P45;<br>CYCLIN A/CDK2-<br>ASSOCIATED PROTEIN P19;<br>SKP1, SKP2, F-BOX, LRR,<br>LEUCINE-RICH REPEAT,<br>SCF, UBIQUITIN, 2 E3,<br>UBIQUITIN PROTEIN<br>LIGASE | TRANSCRIPTION RNA1P;      |
|---------|----------------------|---------------------------------------------------|-------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------|
|         | Compound             |                                                   | NUCLEAR RNA EXPORT<br>FACTOR 1; CHAIN: A, B;                                                                      | NUCLEAR RNA EXPORT<br>FACTOR 1; CHAIN: A, B;                                                       | NUCLEAR RNA EXPORT<br>FACTOR 1; CHAIN: A, B;                                                       | SKP2; CHAIN: A, C, E, G, I, K, M, O; SKP1; CHAIN: B, D, F, H, J, L, N, P;                                                                                                                                | GTPASE-ACTIVATING PROTEIN |
| Table 5 | SEQ<br>FOLD<br>score |                                                   |                                                                                                                   |                                                                                                    |                                                                                                    |                                                                                                                                                                                                          |                           |
| Та      | PMF                  |                                                   | 0.03                                                                                                              | 0.01                                                                                               | 0.17                                                                                               | -0.13                                                                                                                                                                                                    | 0:30                      |
|         | Verify               |                                                   | -0.74                                                                                                             | 0.15                                                                                               | -0.88                                                                                              | 0.26                                                                                                                                                                                                     | 0.22                      |
|         | Psi<br>Blast         |                                                   | 0.0012                                                                                                            | 1.7e-06                                                                                            | 0.0036                                                                                             | 1.4e-09                                                                                                                                                                                                  | 8.5e-13                   |
|         | END                  |                                                   | 571                                                                                                               | 478                                                                                                | 487                                                                                                | <i>578</i>                                                                                                                                                                                               | 487                       |
| •       | START<br>AA          |                                                   | 507                                                                                                               | 385                                                                                                | 441                                                                                                | 363                                                                                                                                                                                                      | 257                       |
|         | CHAIN<br>ID          |                                                   | Ą                                                                                                                 | В                                                                                                  | В                                                                                                  | Ą                                                                                                                                                                                                        | А                         |
|         | PDB<br>ID            |                                                   | 1f01                                                                                                              | 1fo1                                                                                               | 1fo1                                                                                               | 1fqv                                                                                                                                                                                                     | 1yrg                      |
|         | SEQ<br>ID<br>NO:     |                                                   | 1871                                                                                                              | 1871                                                                                               | 1871                                                                                               | 1871                                                                                                                                                                                                     | 1871                      |

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| A A  | Rlact | score  | SCOTE | SEX<br>FOID |        |

| _           |                            |                                                                                                                                                                                                    |                                                                                                                                                                                                                        | · · · · · · · · · · · · · · · · · · ·                                                                                                                                                                                  |                                         |
|-------------|----------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------|
| 45. 45. 45. | PDB annotation             | RANGAP; GTPASE- ACTIVATING PROTEIN FOR SPI1, GTPASE-ACTIVATING PROTEIN, GAP, RNA1P, RANGAP, LRR, LEUCINE- 2 RICH REPEAT PROTEIN, TWINNING, 3 MEROHEDRAL TWINNING, 3 MEROHEDRAL TWINNING MEROHEDRAL | TRANSCRIPTION RNAIP; RANGAP; GTPASE- ACTIVATING PROTEIN FOR SPII, GTPASE-ACTIVATING PROTEIN, GAP, RNAIP, RANGAP, LRR, LEUCINE- 2 RICH REPEAT PROTEIN, TWINNING, HEMIHEDRAL TWINNING, 3 MEROHEDRAL TWINNING, MEROHEDRAL | TRANSCRIPTION RNAIP; RANGAP; GTPASE- ACTIVATING PROTEIN FOR SPI1, GTPASE-ACTIVATING PROTEIN, GAP, RNAIP, RANGAP, LRR, LEUCINE- 2 RICH REPEAT PROTEIN, TWINNING, HEMIHEDRAL TWINNING, 3 MEROHEDRAL TWINNING, MEROHEDRAL | ACETYLATION RNASE INHIBITOR,            |
|             | Compound                   | RNA1_SCHPO; CHAIN: A, B;                                                                                                                                                                           | GTPASE-ACTIVATING PROTEIN<br>RNA1_SCHPO; CHAIN: A, B;                                                                                                                                                                  | GTPASE-ACTIVATING PROTEIN RNA1_SCHPO; CHAIN: A, B;                                                                                                                                                                     | RIBONUCLEASE INHIBITOR;<br>CHAIN: NULL; |
| l able 5    | SEQ<br>FOLD<br>score       |                                                                                                                                                                                                    |                                                                                                                                                                                                                        |                                                                                                                                                                                                                        | 145.84                                  |
| La          | Score                      |                                                                                                                                                                                                    | 0.07                                                                                                                                                                                                                   | 1.00                                                                                                                                                                                                                   |                                         |
|             | Venty                      |                                                                                                                                                                                                    | 0.08                                                                                                                                                                                                                   | 0.48                                                                                                                                                                                                                   |                                         |
|             | Ps1<br>Blast               |                                                                                                                                                                                                    | 3.4e-15                                                                                                                                                                                                                | 5.1e-17                                                                                                                                                                                                                | 1.7e-49                                 |
| 3           | END                        |                                                                                                                                                                                                    | 571                                                                                                                                                                                                                    | 290                                                                                                                                                                                                                    | 591                                     |
| - 1         | SIAKI<br>AA                |                                                                                                                                                                                                    | 296                                                                                                                                                                                                                    | 361                                                                                                                                                                                                                    | 143                                     |
|             | CHAIN                      |                                                                                                                                                                                                    | ∢                                                                                                                                                                                                                      | ¥                                                                                                                                                                                                                      |                                         |
|             | PDB<br>ID                  |                                                                                                                                                                                                    | lyrg                                                                                                                                                                                                                   | lyrg                                                                                                                                                                                                                   | 2bnh                                    |
| 6           | A<br>A<br>B<br>S<br>B<br>S |                                                                                                                                                                                                    | 1871                                                                                                                                                                                                                   | 1871                                                                                                                                                                                                                   | 1871                                    |

|         | PDB annotation |           | RIBONUCLEASE/ANGIOGEN IN INHIBITOR | ACETYLATION, LEUCINE-<br>RICH REPEATS | ACETYLATION RNASE       | INHIBITOR,   | RIBONUCLEASE/ANGIOGEN | IN INHIBITOR | ACELYLATION, LEUCINE-<br>RICH REPEATS | SIGNAL TRANSDUCTION      | PROTEIN PLECKSTRIN, | PHOSPHOLIPASE, INOSITOL | TRISPHOSPHATE, 2 SIGNAL | TRANSDUCTION PROTEIN, | HYDROLASE | SIGNAL TRANSDUCTION      | PROTEIN PLECKSTRIN, | PHOSPHOLIPASE, INOSITOL | TRISPHOSPHATE, 2 SIGNAL | TRANSDUCTION PROTEIN, | HYDROLASE | SIGNAL TRANSDUCTION      | PROTEIN PLECKSTRIN, | PHOSPHOLIPASE, INOSITOL | TRISPHOSPHATE, 2 SIGNAL | TRANSDUCTION PROTEIN, | HYDROLASE | SIGNAL TRANSDUCTION<br>PROTEIN PLECKSTRIN, |  |
|---------|----------------|-----------|------------------------------------|---------------------------------------|-------------------------|--------------|-----------------------|--------------|---------------------------------------|--------------------------|---------------------|-------------------------|-------------------------|-----------------------|-----------|--------------------------|---------------------|-------------------------|-------------------------|-----------------------|-----------|--------------------------|---------------------|-------------------------|-------------------------|-----------------------|-----------|--------------------------------------------|--|
|         | Compound       |           |                                    |                                       | RIBONUCLEASE INHIBITOR; | CHAIN: NULL; |                       |              |                                       | PHOSPHOLIPASE C DELTA-1; | CHAIN: NULL;        |                         |                         |                       |           | PHOSPHOLIPASE C DELTA-1; | CHAIN: NULL;        |                         |                         |                       |           | PHOSPHOLIPASE C DELTA-1; | CHAIN: NULL;        |                         |                         |                       |           | PHOSPHOLIPASE C DELTA-1;<br>CHAIN: NULL;   |  |
| Table 5 | SEQ            | FULD      |                                    |                                       |                         |              |                       |              |                                       |                          |                     |                         |                         |                       |           |                          |                     |                         |                         |                       |           | 65.10                    |                     | -                       |                         |                       |           | 65.10                                      |  |
| Tak     | PMF            | score     |                                    |                                       | 1.00                    |              |                       |              |                                       | 1.00                     |                     |                         |                         |                       |           | 1.00                     |                     |                         |                         |                       |           |                          |                     |                         | -                       |                       |           |                                            |  |
|         | Verify         | score     |                                    |                                       | 0.12                    |              |                       |              |                                       | 0.87                     |                     |                         |                         |                       |           | 0.87                     |                     |                         |                         |                       |           |                          |                     |                         |                         |                       |           |                                            |  |
|         | Psi            | Blast     |                                    |                                       | 1.7e-49                 |              |                       |              |                                       | 3.4e-35                  |                     |                         |                         |                       |           | 3.4e-35                  |                     |                         |                         |                       |           | 3.4e-35                  |                     |                         |                         |                       |           | 3.4e-35                                    |  |
|         | END            | AA        |                                    |                                       | 590                     |              |                       | •            |                                       | 127                      |                     |                         |                         |                       |           | 127                      |                     |                         |                         |                       |           | 128                      |                     |                         |                         | -                     |           | 128                                        |  |
|         | START          | AA        |                                    |                                       | 166                     |              |                       |              |                                       | 12                       |                     |                         |                         |                       |           | 12                       |                     |                         |                         |                       |           | 6                        |                     |                         |                         |                       |           | 6                                          |  |
|         | CHAIN          | <br>A     |                                    |                                       |                         |              |                       |              |                                       |                          |                     |                         |                         |                       |           |                          |                     |                         |                         |                       |           |                          |                     |                         |                         |                       |           |                                            |  |
|         | PDB            | <br>A     |                                    |                                       | 2bnh                    |              |                       |              |                                       | 1mai                     |                     |                         |                         |                       |           | 1mai                     |                     |                         |                         |                       |           | 1mai                     |                     |                         |                         |                       |           | 1mai                                       |  |
|         | SEQ            | ——<br>日 ஜ |                                    |                                       | 1871                    |              |                       |              |                                       | 1886                     |                     |                         |                         |                       |           | 1886                     |                     |                         |                         |                       |           | 1886                     |                     |                         |                         |                       |           | 1886                                       |  |

Table 5

|         | PDB annotation       | PHOSPHOLIPASE, INOSITOL TRISPHOSPHATE, 2 SIGNAL TRANSDUCTION PROTEIN, HYDROLASE | COMPLEX (ZINC<br>FINGER/DNA) COMPLEX<br>(ZINC FINGER/DNA), ZINC<br>FINGER, DNA-BINDING | COMPLEX (ZINC<br>FINGER/DNA) ZINC FINGER,<br>PROTEIN-DNA<br>INTERACTION, PROTEIN<br>DESIGN, 2 CRYSTAL<br>STRUCTURE, COMPLEX<br>(ZINC FINGER/DNA) | COMPLEX (TRANSCRIPTION REGULATION/DNA) COMPLEX (TRANSCRIPTION REGULATION/DNA), RNA POLYMERASE III, 2 TRANSCRIPTION INITIATION, ZINC FINGER PROTEIN | COMPLEX (TRANSCRIPTION<br>REGULATION/DNA) YING-<br>YANG 1; TRANSCRIPTION<br>INITIATION, INITIATOR<br>ELEMENT, YY1, ZINC 2<br>FINGER PROTEIN, DNA- |
|---------|----------------------|---------------------------------------------------------------------------------|----------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------|
|         | Compound             |                                                                                 | QGSR ZINC FINGER PEPTIDE; CHAIN: A; DUPLEX OLIGONUCLEOTIDE BINDING SITE; CHAIN: B, C;  | DNA; CHAIN: A, B, D, E;<br>CONSENSUS ZINC FINGER<br>PROTEIN; CHAIN: C, F, G;                                                                     | TFIIIA; CHAIN: A, D; 5S<br>RIBOSOMAL RNA GENE; CHAIN:<br>B, C, E, F;                                                                               | YY1; CHAIN: C; ADENO-ASSOCIATED VIRUS P5 INITIATOR ELEMENT DNA; CHAIN: A, B;                                                                      |
| Table 5 | SEQ<br>FOLD<br>score |                                                                                 | 88.83                                                                                  | 108.16                                                                                                                                           | 114.66                                                                                                                                             | 96.44                                                                                                                                             |
| Lab     | PMF                  |                                                                                 |                                                                                        |                                                                                                                                                  |                                                                                                                                                    |                                                                                                                                                   |
|         | Verify               |                                                                                 |                                                                                        |                                                                                                                                                  |                                                                                                                                                    |                                                                                                                                                   |
|         | Psi<br>Blast         |                                                                                 | 1.8e-44                                                                                | 1.7e-50                                                                                                                                          | 1.4e-76                                                                                                                                            | 2e-59                                                                                                                                             |
|         | END                  |                                                                                 | 488                                                                                    | 431                                                                                                                                              | 461                                                                                                                                                | 431                                                                                                                                               |
|         | START<br>AA          |                                                                                 | 406                                                                                    | 349                                                                                                                                              | 293                                                                                                                                                | 319                                                                                                                                               |
|         | CHAIN                |                                                                                 | A                                                                                      | U                                                                                                                                                | V                                                                                                                                                  | ပ                                                                                                                                                 |
|         | PDB<br>UD            |                                                                                 | 1a1h                                                                                   | 1mey                                                                                                                                             | 1tf6                                                                                                                                               | 1ubd                                                                                                                                              |
|         | SEQ<br>ID<br>NO:     |                                                                                 | 1898                                                                                   | 1898                                                                                                                                             | 1898                                                                                                                                               | 1898                                                                                                                                              |

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|  | PDB annotation       | PROTEIN RECOGNITION, 3<br>COMPLEX (TRANSCRIPTION<br>REGULATION/DNA) | COMPLEX (DNA-BINDING<br>PROTEIN/DNA) FIVE-<br>FINGER GLI; GLI, ZINC<br>FINGER, COMPLEX (DNA-<br>BINDING PROTEIN/DNA) |   | COMPLEX (ZINC<br>FINGER/DNA) COMPLEX<br>(ZINC FINGER/DNA), ZINC<br>FINGER, DNA-BINDING<br>PROTEIN | COMPLEX (ZINC<br>FINGER/DNA) ZINC FINGER,<br>PROTEIN-DNA                     | INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC<br>FINGER/DNA) ZINC FINGER,<br>PROTEIN-DNA<br>INTERACTION, PROTEIN<br>DESIGN, 2 CRYSTAL<br>STRUCTURE, COMPLEX<br>(ZINC FINGER/DNA) | COMPLEX (ZINC<br>FINGER/DNA) ZINC FINGER,<br>PROTEIN-DNA                     |
|--|----------------------|---------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------|---|---------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------|-----------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------|
|  | Compound             |                                                                     | ZINC FINGER PROTEIN GLI1;<br>CHAIN: A; DNA; CHAIN: C, D;                                                             |   | QGSR ZINC FINGER PEPTIDE;<br>CHAIN: A; DUPLEX<br>OLIGONUCLEOTIDE BINDING<br>SITE; CHAIN: B, C;    | DNA; CHAIN: A, B, D, E;<br>CONSENSUS ZINC FINGER<br>PROTEIN; CHAIN: C, F, G; |                                                                             | DNA; CHAIN: A, B, D, E;<br>CONSENSUS ZINC FINGER<br>PROTEIN; CHAIN: C, F, G;                                                                     | DNA; CHAIN: A, B, D, E;<br>CONSENSUS ZINC FINGER<br>PROTEIN; CHAIN: C, F, G; |
|  | SEQ<br>FOLD<br>score |                                                                     | 107.35                                                                                                               |   |                                                                                                   |                                                                              |                                                                             |                                                                                                                                                  |                                                                              |
|  | PMF                  |                                                                     |                                                                                                                      |   | -0.18                                                                                             | 0.13                                                                         |                                                                             | 0.24                                                                                                                                             | 0.86                                                                         |
|  | Verify<br>score      |                                                                     |                                                                                                                      |   | 0.12                                                                                              | -0.29                                                                        |                                                                             | -0.26                                                                                                                                            | 0.09                                                                         |
|  | Psi<br>Blast         |                                                                     | 6e-74                                                                                                                |   | 5.1e-20                                                                                           | 3.4e-33                                                                      |                                                                             | 6.8e-36                                                                                                                                          | 1.7e-36                                                                      |
|  | END                  |                                                                     | 460                                                                                                                  |   | 185                                                                                               | 186                                                                          |                                                                             | 212                                                                                                                                              | 240                                                                          |
|  | START<br>AA          |                                                                     | 323                                                                                                                  |   | 107                                                                                               | 106                                                                          |                                                                             | 135                                                                                                                                              | 163                                                                          |
|  | CHAIN<br>ID          |                                                                     | A                                                                                                                    |   | ¥                                                                                                 | O                                                                            |                                                                             | O                                                                                                                                                | O                                                                            |
|  | PDB<br>ID            |                                                                     | 2gli                                                                                                                 | - | lalh                                                                                              | lmey                                                                         |                                                                             | 1mey                                                                                                                                             | lmey                                                                         |
|  | SEQ<br>ID<br>NO:     |                                                                     | 1898                                                                                                                 |   | 1937                                                                                              | 1937                                                                         |                                                                             | 1937                                                                                                                                             | 1937                                                                         |

|         | PDB annotation       | INTERACTION, PROTEIN<br>DESIGN, 2 CRYSTAL<br>STRUCTURE, COMPLEX<br>(ZINC FINGER/DNA) | COMPLEX (ZINC<br>FINGER/DNA) ZINC FINGER,<br>PROTEIN-DNA<br>INTERACTION, PROTEIN<br>DESIGN, 2 CRYSTAL<br>STRUCTURE, COMPLEX<br>(ZINC FINGER/DNA) | COMPLEX (ZINC<br>FINGER/DNA) ZINC FINGER,<br>PROTEIN-DNA<br>INTERACTION, PROTEIN<br>DESIGN, 2 CRYSTAL<br>STRUCTURE, COMPLEX<br>(ZINC FINGER/DNA) | COMPLEX (ZINC<br>FINGER/DNA) ZINC FINGER,<br>PROTEIN-DNA<br>INTERACTION, PROTEIN<br>DESIGN, 2 CRYSTAL<br>STRUCTURE, COMPLEX<br>(ZINC FINGER/DNA) | COMPLEX (ZINC<br>FINGER/DNA) ZINC FINGER,<br>PROTEIN-DNA<br>INTERACTION, PROTEIN<br>DESIGN, 2 CRYSTAL<br>STRUCTURE, COMPLEX |
|---------|----------------------|--------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------|
|         | Compound             |                                                                                      | DNA; CHAIN: A, B, D, E;<br>CONSENSUS ZINC FINGER<br>PROTEIN; CHAIN: C, F, G;                                                                     | DNA; CHAIN: A, B, D, E;<br>CONSENSUS ZINC FINGER<br>PROTEIN; CHAIN: C, F, G;                                                                     | DNA; CHAIN: A, B, D, E;<br>CONSENSUS ZINC FINGER<br>PROTEIN; CHAIN: C, F, G;                                                                     | DNA; CHAIN: A, B, D, E;<br>CONSENSUS ZINC FINGER<br>PROTEIN; CHAIN: C, F, G;                                                |
| Table 5 | SEQ<br>FOLD<br>score |                                                                                      |                                                                                                                                                  |                                                                                                                                                  |                                                                                                                                                  |                                                                                                                             |
| Tal     | PMF                  |                                                                                      | 0.99                                                                                                                                             | 0.15                                                                                                                                             | 1.00                                                                                                                                             | 0.99                                                                                                                        |
|         | Verify<br>score      |                                                                                      | 0.38                                                                                                                                             | -0.33                                                                                                                                            | 60.0                                                                                                                                             | 0.08                                                                                                                        |
|         | Psi<br>Blast         |                                                                                      | 6.8e-42                                                                                                                                          | 6e-42                                                                                                                                            | 5.1e-44                                                                                                                                          | 8e-42                                                                                                                       |
|         | END<br>AA            |                                                                                      | 268                                                                                                                                              | 296                                                                                                                                              | 296                                                                                                                                              | 324                                                                                                                         |
|         | START<br>AA          |                                                                                      | 187                                                                                                                                              | 187                                                                                                                                              | 215                                                                                                                                              | 215                                                                                                                         |
|         | CHAIN<br>ID          |                                                                                      | U                                                                                                                                                | O                                                                                                                                                | O                                                                                                                                                | U                                                                                                                           |
|         | PDB<br>ID            |                                                                                      | Imey                                                                                                                                             | Imey                                                                                                                                             | Imey                                                                                                                                             | lmey                                                                                                                        |
|         | SEQ<br>NO:           |                                                                                      | 1937                                                                                                                                             | 1937                                                                                                                                             | 1937                                                                                                                                             | 1937                                                                                                                        |

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|         | PDB annotation       | (ZINC FINGER/DNA) | COMPLEX (ZINC FINGER,                            | PROTEIN-DNA              | INTERACTION, PROTEIN | DESIGN, 2 CRYSTAL | STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC           | FINGER/DNA) ZINC FINGER, | PROTEIN-DNA              | INTERACTION, PROTEIN | DESIGN, 2 CRYSTAL | STRUCTURE, COMPLEX | (ZINC FINGER/DNA) | COMPLEX (ZINC           | FINGER/DNA) ZINC FINGER, | PROTEIN-DNA              | INTERACTION, PROTEIN | DESIGN, 2 CRYSTAL | STRUCTURE, COMPLEX | (ZINC FINGER/DNA) | COMPLEX (ZINC           | FINGER/DNA) ZINC FINGER, | PROTEIN-DNA              | INTERACTION, PROTEIN | DESIGN, 2 CRYSTAL | STRUCTURE, COMPLEX | (ZINC FINGER/DNA) | COMPLEX (ZINC<br>FINGER/DNA) ZINC FINGER,        |
|---------|----------------------|-------------------|--------------------------------------------------|--------------------------|----------------------|-------------------|--------------------------------------|-------------------------|--------------------------|--------------------------|----------------------|-------------------|--------------------|-------------------|-------------------------|--------------------------|--------------------------|----------------------|-------------------|--------------------|-------------------|-------------------------|--------------------------|--------------------------|----------------------|-------------------|--------------------|-------------------|--------------------------------------------------|
|         | Compound             |                   | DNA; CHAIN: A, B, D, E;<br>CONSENSUS ZINC FINGER | PROTEIN; CHAIN: C, F, G; |                      |                   |                                      | DNA; CHAIN: A, B, D, E; | CONSENSUS ZINC FINGER    | PROTEIN; CHAIN: C, F, G; |                      |                   |                    |                   | DNA; CHAIN: A, B, D, E; | CONSENSUS ZINC FINGER    | PROTEIN; CHAIN: C, F, G; |                      |                   |                    |                   | DNA; CHAIN: A, B, D, E; | CONSENSUS ZINC FINGER    | PROTEIN; CHAIN: C, F, G; |                      |                   |                    |                   | DNA; CHAIN: A, B, D, E;<br>CONSENSUS ZINC FINGER |
| Table 5 | SEQ<br>FOLD<br>score |                   |                                                  |                          |                      |                   |                                      |                         |                          |                          |                      |                   |                    |                   |                         |                          |                          |                      |                   |                    |                   |                         |                          |                          |                      |                   |                    |                   |                                                  |
| Tak     | PMF                  |                   | 1.00                                             |                          |                      |                   |                                      | 1.00                    |                          |                          |                      |                   |                    |                   | 1.00                    |                          |                          |                      |                   |                    |                   | 1.00                    |                          |                          |                      |                   |                    |                   | 1.00                                             |
|         | Verify<br>score      |                   | 0.35                                             |                          |                      |                   |                                      | 0.26                    |                          |                          |                      |                   |                    |                   | 0.27                    |                          |                          |                      |                   |                    |                   | 0.07                    |                          |                          |                      |                   |                    |                   | 0.15                                             |
|         | Psi<br>Blast         |                   | 5.1e-45                                          |                          |                      |                   |                                      | 1.5e-45                 |                          |                          |                      |                   | -                  |                   | 8e-46                   |                          |                          |                      |                   |                    |                   | 5.1e-46                 |                          |                          |                      |                   |                    |                   | 1e-46                                            |
|         | END<br>AA            |                   | 324                                              |                          |                      |                   |                                      | 352                     |                          |                          |                      | ·                 |                    |                   | 352                     |                          |                          |                      |                   |                    |                   | 380                     |                          |                          |                      | •                 |                    |                   | 408                                              |
|         | START<br>AA          |                   | 243                                              |                          |                      |                   |                                      | 271                     |                          |                          |                      | -                 |                    |                   | 272                     |                          |                          |                      |                   |                    |                   | 299                     |                          |                          |                      |                   |                    |                   | 327                                              |
|         | CHAIN<br>ID          |                   | C                                                |                          |                      |                   |                                      | C                       |                          |                          |                      |                   |                    |                   | C                       |                          |                          |                      |                   |                    |                   | O                       |                          |                          |                      |                   |                    |                   | 2                                                |
|         | PDB<br>ID            |                   | 1mey                                             |                          |                      |                   |                                      | 1mey                    |                          |                          |                      |                   |                    |                   | 1mey                    |                          |                          |                      |                   |                    |                   | 1mey                    | •                        |                          |                      |                   |                    |                   | 1mey                                             |
|         | SEQ<br>EQ            |                   | 1937                                             |                          |                      |                   |                                      | 1937                    |                          |                          |                      |                   |                    |                   | 1937                    |                          |                          |                      |                   |                    |                   | 1937                    |                          |                          |                      |                   |                    |                   | 1937                                             |

|         |                      | ¬                                                                     |                                                                                                                             |                                                                                                                                   |                                                                                                                                                  |                                                                                                       |
|---------|----------------------|-----------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------|
|         | PDB annotation       | PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX | COMPLEX (ZINC<br>FINGER/DNA) ZINC FINGER,<br>PROTEIN-DNA<br>INTERACTION, PROTEIN<br>DESIGN, 2 CRYSTAL<br>STRUCTURE, COMPLEX | COMPLEX (ZINC FINGER/DNA) ZINC FINGER, PROTEIN-DNA INTERACTION, PROTEIN DESIGN, 2 CRYSTAL STRUCTURE, COMPLEX (ZINC FINGER D.N.A.) | COMPLEX (ZINC<br>FINGER/DNA) ZINC FINGER,<br>PROTEIN-DNA<br>INTERACTION, PROTEIN<br>DESIGN, 2 CRYSTAL<br>STRUCTURE, COMPLEX<br>(ZINC FINGER/DNA) | COMPLEX (ZINC<br>FINGER/DNA) ZINC FINGER,<br>PROTEIN-DNA<br>INTERACTION, PROTEIN<br>DESIGN, 2 CRYSTAL |
|         | Compound             | PROTEIN; CHAIN: C, F, G;                                              | DNA; CHAIN: A, B, D, E;<br>CONSENSUS ZINC FINGER<br>PROTEIN; CHAIN: C, F, G;                                                | DNA; CHAIN: A, B, D, E;<br>CONSENSUS ZINC FINGER<br>PROTEIN; CHAIN: C, F, G;                                                      | DNA; CHAIN: A, B, D, E;<br>CONSENSUS ZINC FINGER<br>PROTEIN; CHAIN: C, F, G;                                                                     | DNA; CHAIN: A, B, D, E;<br>CONSENSUS ZINC FINGER<br>PROTEIN; CHAIN: C, F, G;                          |
| Table 5 | SEQ<br>FOLD<br>score |                                                                       |                                                                                                                             |                                                                                                                                   |                                                                                                                                                  |                                                                                                       |
| Ta      | PMF                  |                                                                       | 1.00                                                                                                                        | 1.00                                                                                                                              | 1.00                                                                                                                                             | 1.00                                                                                                  |
|         | Verify<br>score      |                                                                       | 0.14                                                                                                                        | 0.59                                                                                                                              | 09.0                                                                                                                                             | 0.57                                                                                                  |
|         | Psi<br>Blast         |                                                                       | 5.1e-47                                                                                                                     | 8.5e-47                                                                                                                           | 3.4e-47                                                                                                                                          | 1.7e-48                                                                                               |
|         | END                  |                                                                       | 436                                                                                                                         | 464                                                                                                                               | 492                                                                                                                                              | 520                                                                                                   |
|         | START<br>AA          |                                                                       | 355                                                                                                                         | 383                                                                                                                               | 411                                                                                                                                              | 439                                                                                                   |
|         | CHAIN                |                                                                       | U                                                                                                                           | O                                                                                                                                 | O                                                                                                                                                | O                                                                                                     |
| 5       | PDB<br>D             |                                                                       | 1mey                                                                                                                        | 1mey                                                                                                                              | 1mey                                                                                                                                             | Imey                                                                                                  |
| i i     | A G S                |                                                                       | 1937                                                                                                                        | 1937                                                                                                                              | 1937                                                                                                                                             | 1937                                                                                                  |

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|         |                      |                                      |                         |                          |                          |                      |                   |                    |                   |                         |                          |                          |                      |                   |                    |                   |                         |                          |                          |                      | _                 |                    |                   |                         |                          |                          |                      |                   |                    |                   |                         |
|---------|----------------------|--------------------------------------|-------------------------|--------------------------|--------------------------|----------------------|-------------------|--------------------|-------------------|-------------------------|--------------------------|--------------------------|----------------------|-------------------|--------------------|-------------------|-------------------------|--------------------------|--------------------------|----------------------|-------------------|--------------------|-------------------|-------------------------|--------------------------|--------------------------|----------------------|-------------------|--------------------|-------------------|-------------------------|
|         | PDB annotation       | STRUCTURE, COMPLEX (ZINC FINGER/DNA) | COMPLEX (ZINC           | FINGER/DNA) ZINC FINGER, | PROTEIN-DNA              | INTERACTION, PROTEIN | DESIGN, 2 CRYSTAL | STRUCTURE, COMPLEX | (ZINC FINGER/DNA) | COMPLEX (ZINC           | FINGER/DNA) ZINC FINGER, | PROTEIN-DNA              | INTERACTION, PROTEIN | DESIGN, 2 CRYSTAL | STRUCTURE, COMPLEX | (ZINC FINGER/DNA) | COMPLEX (ZINC           | FINGER/DNA) ZINC FINGER, | PROTEIN-DNA              | INTERACTION, PROTEIN | DESIGN, 2 CRYSTAL | STRUCTURE, COMPLEX | (ZINC FINGER/DNA) | COMPLEX (ZINC           | FINGER/DNA) ZINC FINGER, | PROTEIN-DNA              | INTERACTION, PROTEIN | DESIGN, 2 CRYSTAL | STRUCTURE, COMPLEX | (ZINC FINGER/DNA) | COMPLEX (ZINC           |
|         | Compound             |                                      | DNA; CHAIN: A, B, D, E; | CONSENSUS ZINC FINGER    | PROTEIN; CHAIN: C, F, G; |                      |                   |                    |                   | DNA; CHAIN: A, B, D, E; | CONSENSUS ZINC FINGER    | PROTEIN; CHAIN: C, F, G; |                      |                   |                    |                   | DNA; CHAIN: A, B, D, E; | CONSENSUS ZINC FINGER    | PROTEIN; CHAIN: C, F, G; |                      |                   |                    |                   | DNA; CHAIN: A, B, D, E; | CONSENSUS ZINC FINGER    | PROTEIN; CHAIN: C, F, G; |                      |                   |                    |                   | DNA; CHAIN: A, B, D, E; |
| Table 5 | SEQ<br>FOLD<br>score |                                      |                         |                          |                          |                      |                   |                    |                   |                         |                          |                          |                      |                   |                    |                   |                         |                          |                          |                      |                   |                    |                   |                         |                          |                          |                      |                   |                    |                   | 103.75                  |
| Tal     | PMF                  |                                      | 1.00                    |                          |                          |                      |                   |                    |                   | 1.00                    |                          |                          |                      |                   |                    |                   | 1.00                    |                          |                          |                      |                   |                    |                   | 1.00                    |                          |                          |                      |                   |                    |                   |                         |
|         | Verify<br>score      |                                      | 0.57                    |                          |                          |                      |                   |                    |                   | 0.62                    |                          |                          |                      |                   |                    |                   | 0.34                    |                          |                          |                      |                   |                    |                   | 0.61                    |                          |                          |                      |                   |                    |                   |                         |
|         | Psi<br>Blast         |                                      | 3.4e-49                 |                          |                          |                      |                   |                    |                   | 1e-49                   |                          |                          |                      |                   |                    |                   | 3.4e-50                 |                          |                          |                      |                   |                    |                   | 1.4e-50                 |                          |                          |                      |                   |                    |                   | 1e-50                   |
|         | END                  |                                      | 548                     |                          |                          |                      |                   |                    |                   | 576                     |                          |                          |                      |                   |                    |                   | 604                     |                          |                          |                      |                   |                    |                   | 632                     |                          |                          |                      |                   |                    |                   | 633                     |
|         | START<br>AA          |                                      | 467                     |                          |                          |                      |                   |                    |                   | 495                     |                          |                          |                      |                   |                    |                   | 523                     |                          |                          |                      |                   |                    |                   | 551                     |                          |                          |                      |                   |                    |                   | 551                     |
|         | CHAIN                |                                      | C                       |                          |                          |                      |                   |                    |                   | ၁                       |                          |                          |                      |                   |                    |                   | S                       |                          |                          |                      |                   |                    |                   | ၁                       |                          |                          |                      |                   |                    |                   | C                       |
|         | PDB<br>ID            |                                      | 1mey                    |                          |                          |                      |                   |                    |                   | 1mey                    |                          |                          |                      |                   |                    |                   | 1mey                    | `                        |                          | -                    |                   |                    |                   | 1 mey                   |                          |                          |                      |                   |                    |                   | 1mey                    |
|         | SEQ<br>ID<br>NO:     |                                      | 1937                    |                          |                          |                      |                   |                    |                   | 1937                    |                          |                          |                      |                   |                    |                   | 1937                    |                          |                          |                      |                   |                    |                   | 1937                    |                          |                          |                      |                   |                    |                   | 1937                    |

| _       |                 | ·                                                 |                      |                   |                                       | _                    |                          |                          |                      |                   |                    |                   |                         |                          |                          |                      |                   |                    |                   |                         |                          |                          |                      |                   |                    |                   |                         |                          |                                       | 1 |
|---------|-----------------|---------------------------------------------------|----------------------|-------------------|---------------------------------------|----------------------|--------------------------|--------------------------|----------------------|-------------------|--------------------|-------------------|-------------------------|--------------------------|--------------------------|----------------------|-------------------|--------------------|-------------------|-------------------------|--------------------------|--------------------------|----------------------|-------------------|--------------------|-------------------|-------------------------|--------------------------|---------------------------------------|---|
|         | PDB annotation  | FINGER/DNA) ZINC FINGER,<br>PROTEIN-DNA           | INTERACTION, PROTEIN | DESIGN, 2 CRYSTAL | STRUCTURE, COMPLEX (ZINC FINGER (DNA) | COMPLEX (ZINC        | FINGER/DNA) ZINC FINGER, | PROTEIN-DNA              | INTERACTION, PROTEIN | DESIGN, 2 CRYSTAL | STRUCTURE, COMPLEX | (ZINC FINGER/DNA) | COMPLEX (ZINC           | FINGER/DNA) ZINC FINGER, | PROTEIN-DNA              | INTERACTION, PROTEIN | DESIGN, 2 CRYSTAL | STRUCTURE, COMPLEX | (ZINC FINGER/DNA) | COMPLEX (ZINC           | FINGER/DNA) ZINC FINGER, | PROTEIN-DNA              | INTERACTION, PROTEIN | DESIGN, 2 CRYSTAL | STRUCTURE, COMPLEX | (ZINC FINGER/DNA) | COMPLEX (ZINC           | FINGER/DNA) ZINC FINGER, | PROTEIN-DNA<br>  INTERACTION. PROTEIN |   |
|         | Compound        | CONSENSUS ZINC FINGER<br>PROTEIN; CHAIN: C, F, G; |                      |                   |                                       | DNA: CHAIN: A R D F. | CONSENSUS ZINC FINGER    | PROTEIN; CHAIN: C, F, G; |                      |                   |                    |                   | DNA; CHAIN: A, B, D, E; | CONSENSUS ZINC FINGER    | PROTEIN; CHAIN: C, F, G; |                      |                   |                    |                   | DNA; CHAIN: A, B, D, E; | CONSENSUS ZINC FINGER    | PROTEIN; CHAIN: C, F, G; |                      |                   |                    |                   | DNA; CHAIN: A, B, D, E; | CONSENSUS ZINC FINGER    | PROTEIN; CHAIN: C, F, G;              |   |
| Table 5 | SEQ<br>FOLD     |                                                   |                      |                   |                                       |                      |                          |                          |                      |                   |                    |                   |                         |                          |                          |                      |                   |                    |                   |                         |                          |                          |                      |                   |                    |                   |                         |                          |                                       |   |
| Tal     | PMF             |                                                   |                      |                   |                                       | 1 00                 | 7.7                      |                          |                      |                   |                    |                   | 1.00                    |                          |                          |                      |                   |                    |                   | 1.00                    |                          |                          |                      |                   |                    |                   | 1.00                    |                          |                                       |   |
|         | Verify<br>score |                                                   |                      |                   |                                       | 99 0                 | 0.00                     |                          |                      |                   |                    |                   | 0.35                    |                          |                          |                      |                   |                    |                   | 0.28                    |                          |                          |                      |                   |                    |                   | 0.36                    |                          |                                       |   |
|         | Psi<br>Blast    |                                                   |                      |                   |                                       | 10.50                | 00-21                    |                          |                      |                   |                    |                   | 1e-50                   |                          |                          |                      |                   |                    |                   | 1.7e-50                 |                          |                          |                      |                   |                    |                   | 1.7e-50                 |                          |                                       |   |
|         | END             |                                                   | -                    |                   |                                       | 099                  |                          |                          |                      |                   |                    |                   | 716                     |                          |                          |                      |                   |                    |                   | 744                     |                          |                          |                      |                   |                    |                   | 772                     |                          |                                       |   |
|         | START           |                                                   |                      |                   |                                       | 670                  | 66                       |                          |                      |                   |                    |                   | 635                     |                          |                          |                      |                   |                    |                   | 663                     |                          |                          |                      |                   |                    |                   | 1691                    |                          |                                       |   |
|         | CHAIN           |                                                   |                      |                   |                                       | ر                    | ر                        |                          |                      |                   |                    |                   | C                       |                          |                          |                      |                   |                    |                   | ၁                       |                          |                          |                      |                   |                    |                   | C                       |                          |                                       |   |
|         | PDB<br>ID       |                                                   |                      |                   |                                       | 120017               | uncy                     |                          |                      |                   | 7                  |                   | 1mey                    |                          |                          |                      |                   |                    |                   | 1mey                    |                          |                          |                      |                   |                    |                   | 1mey                    |                          |                                       |   |
|         | SEQ<br>D        |                                                   |                      |                   |                                       | 1027                 | 1561                     |                          |                      |                   |                    |                   | 1937                    |                          |                          |                      |                   |                    |                   | 1937                    |                          |                          |                      |                   |                    |                   | 1937                    |                          |                                       |   |

|         | PDB annotation |          | DESIGN, 2 CRYSTAL | (ZINC FINGER/DNA) | COMPLEX (ZINC           | FINGER/DNA) ZINC FINGER, | PROTEIN-DNA              | INTERACTION, PROTEIN | DESIGN, 2 CRYSTAL | STRUCTURE, COMPLEX | (ZINC FINGER/DNA) | COMPLEX (ZINC           | FINGER/DNA) ZINC FINGER, | PROTEIN-DNA              | INTERACTION, PROTEIN                  | DESIGN, 2 CRYSTAL | STRUCTURE, COMPLEX | (ZINC FINGER/DNA) | COMPLEX (TRANSCRIPTION  | REGULATION/DNA)            | COMPLEX (TRANSCRIPTION | REGULATION/DNA), RNA | POLYMERASE III, 2 | TRANSCRIPTION | INITIATION, ZINC FINGER | PROTEIN | COMPLEX (TRANSCRIPTION  | REGULATION/DNA)            | COMPLEX (TRANSCRIPTION | REGULATION/DNA), RNA | POLYMERASE III, 2<br>TRANSCRIPTION |
|---------|----------------|----------|-------------------|-------------------|-------------------------|--------------------------|--------------------------|----------------------|-------------------|--------------------|-------------------|-------------------------|--------------------------|--------------------------|---------------------------------------|-------------------|--------------------|-------------------|-------------------------|----------------------------|------------------------|----------------------|-------------------|---------------|-------------------------|---------|-------------------------|----------------------------|------------------------|----------------------|------------------------------------|
|         | Compound       |          |                   |                   | DNA; CHAIN: A, B, D, E; | CONSENSUS ZINC FINGER    | PROTEIN; CHAIN: C, F, G; |                      |                   |                    |                   | DNA; CHAIN: A, B, D, E; | CONSENSUS ZINC FINGER    | PROTEIN; CHAIN: C, F, G; |                                       |                   |                    |                   | TFIIIA; CHAIN: A, D; 5S | RIBOSOMAL RNA GENE; CHAIN: | B, C, E, F;            |                      |                   |               |                         |         | TFIIIA; CHAIN: A, D; 5S | RIBOSOMAL RNA GENE; CHAIN: | B, C, E, F;            |                      |                                    |
| Table 5 | SEQ            | FOLD     |                   |                   |                         |                          |                          |                      |                   |                    |                   |                         |                          |                          |                                       |                   |                    |                   |                         |                            |                        |                      |                   |               |                         |         |                         |                            |                        |                      |                                    |
| Tal     | PMF            | score    |                   |                   | 0.93                    |                          |                          |                      |                   |                    |                   | 0.42                    |                          |                          |                                       |                   |                    |                   | 96.0                    |                            |                        |                      |                   |               |                         |         | 0.82                    |                            |                        |                      |                                    |
|         | Verify         | score    |                   |                   | 0.05                    |                          |                          |                      |                   |                    |                   | -0.14                   |                          |                          |                                       |                   |                    |                   | 80.0                    |                            |                        |                      |                   |               |                         |         | -0.07                   |                            |                        |                      |                                    |
|         | Psi            | Blast    |                   |                   | 1.7e-40                 |                          |                          |                      |                   |                    |                   | 5.1e-09                 |                          |                          |                                       |                   |                    |                   | 3.4e-34                 |                            |                        |                      |                   |               |                         |         | 69-99                   |                            |                        |                      |                                    |
|         | END            | ΑA       |                   |                   | 785                     |                          |                          |                      |                   |                    |                   | 212                     |                          |                          |                                       |                   |                    |                   | 338                     |                            |                        |                      |                   |               |                         |         | 352                     |                            |                        |                      |                                    |
|         | START          | AA       |                   |                   | 719                     |                          |                          | •                    |                   |                    |                   | 185                     |                          |                          | · · · · · · · · · · · · · · · · · · · |                   |                    |                   | 188                     |                            |                        |                      |                   |               |                         |         | 188                     |                            |                        |                      |                                    |
|         | CHAIN          | А        | ·                 |                   | C                       |                          |                          |                      |                   |                    |                   | G                       |                          |                          |                                       |                   |                    |                   | A                       |                            |                        |                      |                   |               |                         |         | A                       |                            |                        |                      |                                    |
|         | PDB            | <u> </u> |                   | _                 | 1mey                    |                          |                          |                      |                   |                    |                   | 1mey                    |                          |                          |                                       |                   |                    |                   | 1tf6                    |                            |                        | •                    |                   |               |                         |         | 1tf6                    |                            |                        |                      |                                    |
|         | SEQ            | A Š      |                   |                   | 1937                    |                          |                          |                      |                   |                    |                   | 1937                    |                          |                          |                                       | ×                 |                    |                   | 1937                    |                            |                        |                      |                   |               |                         |         | 1937                    |                            |                        |                      |                                    |

|         | PDB annotation | INITIATION, ZINC FINGER | COMPLEX (TRANSCRIPTION | KEGULATION/DNA)     | REGULATION/DNA), RNA | POLYMERASE III, 2 | TRANSCRIPTION INITIATION ZINC FINGER | PROTEIN | COMPLEX (TRANSCRIPTION  | REGULATION/DNA)     | COMPLEX (TRANSCRIPTION | REGULATION/DNA), RNA | POLYMERASE III, 2 | TRANSCRIPTION | INITIATION, ZINC FINGER | PROTEIN | COMPLEX (TRANSCRIPTION  | REGULATION/DNA)            | COMPLEX (TRANSCRIPTION | REGULATION/DNA), KNA | POLYMERASE III, 2 | TRANSCRIPTION | INITIATION, ZINC FINGER | PROTEIN | COMPLEX (TRANSCRIPTION  | REGULATION/DNA)            | COMPLEX (TRANSCRIPTION | REGULATION/DNA), KNA<br>POLYMERASE III, 2 |  |
|---------|----------------|-------------------------|------------------------|---------------------|----------------------|-------------------|--------------------------------------|---------|-------------------------|---------------------|------------------------|----------------------|-------------------|---------------|-------------------------|---------|-------------------------|----------------------------|------------------------|----------------------|-------------------|---------------|-------------------------|---------|-------------------------|----------------------------|------------------------|-------------------------------------------|--|
|         | Compound       |                         |                        | AL RNA GENE; CHAIN: | D, C, E, F,          |                   |                                      |         | TFIIIA; CHAIN: A, D; 5S | AL RNA GENE; CHAIN: | B, C, E, F;            |                      |                   |               |                         |         | TFIIIA; CHAIN: A, D; 5S | RIBOSOMAL RNA GENE; CHAIN: | B, C, E, F;            |                      |                   |               |                         |         | TFIIIA; CHAIN: A, D; 5S | RIBOSOMAL RNA GENE; CHAIN: | B, C, E, F;            |                                           |  |
| Table 5 | SEQ<br>FOLD    | score                   |                        |                     |                      |                   |                                      |         |                         |                     |                        |                      |                   |               |                         | •       |                         |                            |                        |                      |                   |               |                         |         |                         |                            |                        |                                           |  |
| Tał     | PMF<br>score   |                         | 1.00                   |                     |                      |                   |                                      |         | 66.0                    |                     |                        |                      |                   |               |                         |         | 1.00                    |                            |                        |                      |                   |               |                         |         | 0.99                    |                            |                        |                                           |  |
|         | Verify score   |                         | -0.12                  |                     |                      |                   |                                      |         | -0.05                   |                     |                        |                      |                   |               |                         |         | -0.18                   |                            |                        |                      |                   |               |                         |         | 0.12                    |                            |                        |                                           |  |
|         | Psi<br>Blast   |                         | 3.4e-34                |                     |                      |                   |                                      |         | 1.2e-72                 |                     |                        |                      |                   | _             |                         |         | 3.4e-35                 |                            |                        |                      |                   |               |                         |         | 3.4e-36                 |                            |                        |                                           |  |
|         | END<br>AA      |                         | 417                    |                     |                      |                   |                                      |         | 436                     |                     |                        |                      |                   |               |                         |         | 473                     |                            |                        |                      |                   |               |                         |         | 501                     |                            |                        |                                           |  |
|         | START<br>AA    |                         | 272                    |                     |                      |                   |                                      |         | 272                     |                     |                        |                      |                   |               |                         |         | 328                     |                            |                        |                      |                   |               |                         |         | 356                     |                            |                        |                                           |  |
|         | CHAIN          |                         | A                      |                     |                      |                   |                                      |         | A                       |                     |                        |                      |                   |               |                         |         | A                       |                            |                        |                      |                   |               |                         |         | A                       |                            |                        |                                           |  |
|         | PDB            |                         | 1tf6                   |                     |                      |                   |                                      |         | 1tf6                    |                     |                        |                      |                   |               |                         |         | 1tf6                    |                            |                        |                      |                   |               |                         |         | 1tf6                    |                            |                        |                                           |  |
|         | SEQ            | NO:                     | 1937                   |                     |                      |                   |                                      |         | 1937                    |                     |                        |                      |                   |               |                         |         | 1937                    |                            |                        |                      |                   |               |                         |         | 1937                    |                            |                        |                                           |  |

|         | PDB annotation |          | TRANSCRIPTION<br>INITIATION, ZINC FINGER<br>PROTEIN | COMPLEX (TRANSCRIPTION REGULATION/DNA)                | COMPLEX (TRANSCRIPTION | POLYMERASE III, 2 | TRANSCRIPTION | INITIATION, ZINC FINGER<br>PROTEIN | COMPLEX (TRANSCRIPTION  | REGULATION/DNA)            | COMPLEX (TRANSCRIPTION | REGULATION/DNA), RNA | POLYMERASE III, 2 | TRANSCRIPTION | INITIATION, ZINC FINGER | PROTEIN | COMPLEX (TRANSCRIPTION  | REGULATION/DNA)            | COMPLEX (TRANSCRIPTION | REGULATION/DNA), RNA | POLYMERASE III, 2 | TRANSCRIPTION | INITIATION, ZINC FINGER | PROTEIN | COMPLEX (TRANSCRIPTION  | REGULATION/DNA)            | COMPLEX (IKANSCKIPIION<br>REGULATION/DNA), RNA |  |
|---------|----------------|----------|-----------------------------------------------------|-------------------------------------------------------|------------------------|-------------------|---------------|------------------------------------|-------------------------|----------------------------|------------------------|----------------------|-------------------|---------------|-------------------------|---------|-------------------------|----------------------------|------------------------|----------------------|-------------------|---------------|-------------------------|---------|-------------------------|----------------------------|------------------------------------------------|--|
|         |                |          | TRA<br>INIT<br>PRO                                  |                                                       | CON                    | POL               | TRA           | INIT                               | <del></del>             |                            | CON                    | REG                  | POL               | TRA           | IN I                    | PRO     |                         |                            | <u> </u>               | REG                  | POL               | TRA           |                         | PRO     |                         |                            | S S                                            |  |
|         | Compound       |          |                                                     | TFIIIA; CHAIN: A, D; 5S<br>RIBOSOMAL RNA GENE; CHAIN: | B, C, E, F;            |                   |               |                                    | TFIIIA; CHAIN: A, D; 5S | RIBOSOMAL RNA GENE; CHAIN: | B,C,E,F;               |                      |                   |               |                         |         | TFIIIA; CHAIN: A, D; 5S | RIBOSOMAL RNA GENE; CHAIN: | B, C, E, F;            |                      |                   |               |                         |         | TFIIIA; CHAIN: A, D; 5S | RIBOSOMAL RNA GENE; CHAIN: | B, C, E, F;                                    |  |
| Table 5 | SEQ            | FOLD     |                                                     |                                                       |                        |                   |               |                                    |                         |                            |                        |                      |                   |               |                         |         |                         |                            |                        |                      |                   |               |                         |         |                         |                            | 21.10                                          |  |
| Tal     | PMF            | score    |                                                     | 1.00                                                  |                        |                   |               |                                    | 1.00                    |                            |                        |                      |                   |               |                         |         | 1.00                    |                            |                        |                      |                   |               |                         |         | 1.00                    |                            |                                                |  |
|         | Verify         | score    |                                                     | -0.12                                                 |                        |                   |               |                                    | 0.42                    |                            |                        |                      |                   |               |                         |         | 90.0                    |                            |                        |                      |                   |               |                         |         | 0.01                    |                            |                                                |  |
|         | Psi            | Blast    |                                                     | 4e-71                                                 |                        |                   |               |                                    | 6.8e-37                 |                            |                        |                      |                   |               |                         |         | 2e-73                   |                            |                        |                      |                   |               |                         |         | 2e-73                   |                            |                                                |  |
|         | END            | ΑA       |                                                     | 576                                                   |                        |                   |               |                                    | 613                     |                            |                        |                      |                   |               |                         |         | 632                     |                            |                        |                      |                   |               |                         |         | 716                     |                            |                                                |  |
|         | START          | AA       |                                                     | 412                                                   |                        |                   |               |                                    | 468                     |                            |                        |                      |                   |               |                         |         | 468                     |                            |                        |                      |                   |               |                         |         | 552                     |                            |                                                |  |
|         | CHAIN          |          |                                                     | A                                                     |                        |                   | -1-           |                                    | A                       |                            |                        |                      |                   |               |                         |         | A                       |                            |                        |                      |                   |               |                         |         | A                       |                            |                                                |  |
|         | PDB            | <u> </u> |                                                     | 1tf6                                                  |                        |                   |               |                                    | 1tf6                    |                            |                        | =                    |                   |               |                         |         | 1tf6                    |                            |                        |                      |                   |               |                         |         | 1tf6                    |                            |                                                |  |
|         | SEQ            | A Ö      |                                                     | 1937                                                  |                        |                   |               |                                    | 1937                    | -                          |                        |                      |                   |               |                         |         | 1937                    |                            |                        |                      |                   |               |                         |         | 1937                    |                            |                                                |  |

|         | PDB annotation       | POLYMERASE III, 2<br>TRANSCRIPTION<br>INITIATION, ZINC FINGER | COMPLEX (TRANSCRIPTION REGULATION/DNA) COMPLEX (TRANSCRIPTION REGULATION/DNA), RNA POLYMERASE III, 2 TRANSCRIPTION INTIATION, ZINC FINGER | COMPLEX (TRANSCRIPTION REGULATION/DNA) COMPLEX (TRANSCRIPTION REGULATION/DNA), RNA POLYMERASE III, 2 TRANSCRIPTION INITIATION, ZINC FINGER PROTEIN | COMPLEX (TRANSCRIPTION REGULATION/DNA) COMPLEX (TRANSCRIPTION REGULATION/DNA), RNA POLYMERASE III, 2 TRANSCRIPTION INTIATION, ZINC FINGER PROTEIN | COMPLEX (TRANSCRIPTION REGULATION/DNA) COMPLEX (TRANSCRIPTION        |
|---------|----------------------|---------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------|
|         | Compound             |                                                               | TFIIIA; CHAIN: A, D; 5S<br>RIBOSOMAL RNA GENE; CHAIN:<br>B, C, E, F;                                                                      | TFIIIA; CHAIN: A, D; 5S<br>RIBOSOMAL RNA GENE; CHAIN:<br>B, C, E, F;                                                                               | TFIIIA; CHAIN: A, D; 5S<br>RIBOSOMAL RNA GENE; CHAIN:<br>B, C, E, F;                                                                              | TFIIIA; CHAIN: A, D; 5S<br>RIBOSOMAL RNA GENE; CHAIN:<br>B, C, E, F; |
| Table 5 | SEQ<br>FOLD<br>score |                                                               | 108.49                                                                                                                                    |                                                                                                                                                    |                                                                                                                                                   |                                                                      |
| la      | PMF                  |                                                               |                                                                                                                                           | 1.00                                                                                                                                               | 96.0                                                                                                                                              | 96.0                                                                 |
| ;       | Venty                |                                                               |                                                                                                                                           | 0.25                                                                                                                                               | 0.11                                                                                                                                              | 0.27                                                                 |
|         | Psi<br>Blast         |                                                               | 2e-73                                                                                                                                     | 6.8e-38                                                                                                                                            | 2e-71                                                                                                                                             | 3.4e-37                                                              |
| T. C.   | AA                   |                                                               | 742                                                                                                                                       | 725                                                                                                                                                | 772                                                                                                                                               | 785                                                                  |
|         | AA                   |                                                               | 579                                                                                                                                       | 580                                                                                                                                                | 809                                                                                                                                               | 636                                                                  |
| CITABL  | D D                  |                                                               | A                                                                                                                                         | A                                                                                                                                                  | Ą                                                                                                                                                 | A                                                                    |
| מעמ     | E D                  |                                                               | 11f6                                                                                                                                      | 1476                                                                                                                                               | 1116                                                                                                                                              | 1tf6                                                                 |
| CEO     | N B S                |                                                               | 1937                                                                                                                                      | 1937                                                                                                                                               | 1937                                                                                                                                              | 1937                                                                 |

|         | PDB annotation  | REGULATION/DNA), RNA<br>POLYMERASE III, 2<br>TRANSCRIPTION<br>INITIATION, ZINC FINGER<br>PROTEIN | COMPLEX (TRANSCRIPTION REGULATION/DNA) YING-YANG 1; TRANSCRIPTION INITIATION ELEMENT, YY1, ZINC 2 FINGER PROTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULATION/DNA) | COMPLEX (TRANSCRIPTION REGULATION/DNA) YING-YANG 1; TRANSCRIPTION INITIATION INITIATOR ELEMENT, YY1, ZINC 2 FINGER PROTEIN, DNA-PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRIPTION REGULATION/DNA) | COMPLEX (TRANSCRIPTION<br>REGULATION/DNA) YING-<br>YANG 1; TRANSCRIPTION<br>INITIATION, INITIATOR<br>ELEMENT, YY1, ZINC 2<br>FINGER PROTEIN, DNA-<br>PROTEIN RECOGNITION, 3<br>COMPLEX (TRANSCRIPTION |
|---------|-----------------|--------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
|         | Compound        |                                                                                                  | YYI; CHAIN: C; ADENO-<br>ASSOCIATED VIRUS P5<br>INITIATOR ELEMENT DNA;<br>CHAIN: A, B;                                                                                              | YY1; CHAIN: C; ADENO-<br>ASSOCIATED VIRUS P5<br>INITIATOR ELEMENT DNA;<br>CHAIN: A, B;                                                                                                        | YYI; CHAIN: C; ADENO-<br>ASSOCIATED VIRUS P5<br>INITIATOR ELEMENT DNA;<br>CHAIN: A, B;                                                                                                                |
| Table 5 | SEQ<br>FOLD     |                                                                                                  |                                                                                                                                                                                     |                                                                                                                                                                                               |                                                                                                                                                                                                       |
| Tal     | PMF             |                                                                                                  | 0.11                                                                                                                                                                                | 0.75                                                                                                                                                                                          | 0.94                                                                                                                                                                                                  |
|         | Verify<br>score |                                                                                                  | -0.45                                                                                                                                                                               | 0.12                                                                                                                                                                                          | -0.19                                                                                                                                                                                                 |
|         | Psi<br>Blast    |                                                                                                  | 5.1e-24                                                                                                                                                                             | 3.4e-28                                                                                                                                                                                       | 6.8e-31                                                                                                                                                                                               |
|         | END             |                                                                                                  | 212                                                                                                                                                                                 | 268                                                                                                                                                                                           | 296                                                                                                                                                                                                   |
|         | START<br>AA     |                                                                                                  | 112                                                                                                                                                                                 | 166                                                                                                                                                                                           | 195                                                                                                                                                                                                   |
|         | CHAIN           |                                                                                                  | ن<br>ن                                                                                                                                                                              | U                                                                                                                                                                                             | U                                                                                                                                                                                                     |
|         | PDB<br>ID       | 3                                                                                                | 1ubd                                                                                                                                                                                | 1ubd                                                                                                                                                                                          | 1ubd                                                                                                                                                                                                  |
|         | SEQ<br>FD SEQ   | 2                                                                                                | 1937                                                                                                                                                                                | 1937                                                                                                                                                                                          | 1937                                                                                                                                                                                                  |

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|---------|----------------|-------------|-----------------|----------------------------------------------|------------------------|--------------------|----------------------|------------------------|------------------------------------------|------------------------|-----------------------|------------------------|-----------------------|----------------------|----------------------|------------------------|------------------------|-----------------|------------------------|-----------------------|------------------------|-----------------------|----------------------|----------------------|------------------------|------------------------|-----------------|------------------------|-----------------------|------------------------|
|         | PDB annotation |             | REGULATION/DNA) | COMPLEX (TRANSCRIPTION REGULATIONDNA) YING-  | YANG 1; TRANSCRIPTION  | FIRMENT VY1 ZINC 2 | FINGER PROTEIN, DNA- | PROTEIN RECOGNITION, 3 | COMPLEX (TRANSCRIPTION   REGULATION/DNA) | COMPLEX (TRANSCRIPTION | REGULATION/DNA) YING- | YANG 1; TRANSCRIPTION  | INITIATION, INITIATOR | ELEMENT, YY1, ZINC 2 | FINGER PROTEIN, DNA- | PROTEIN RECOGNITION, 3 | COMPLEX (TRANSCRIPTION | REGULATION/DNA) | COMPLEX (TRANSCRIPTION | REGULATION/DNA) YING- | YANG 1; TRANSCRIPTION  | INITIATION, INITIATOR | ELEMENT, YY1, ZINC 2 | FINGER PROTEIN, DNA- | PROTEIN RECOGNITION, 3 | COMPLEX (TRANSCRIPTION | REGULATION/DNA) | COMPLEX (TRANSCRIPTION | REGULATION/DNA) YING- | YANG I; IKANSCKIP IION |
|         | Compound       |             |                 | YY1; CHAIN: C; ADENO-<br>ASSOCIATED VIRUS P5 | INITIATOR ELEMENT DNA; | CHAIN: A, B;       |                      |                        |                                          | YY1; CHAIN: C; ADENO-  | ASSOCIATED VIRUS P5   | INITIATOR ELEMENT DNA; | CHAIN: A, B;          |                      |                      |                        |                        |                 | YY1; CHAIN: C; ADENO-  | ASSOCIATED VIRUS P5   | INITIATOR ELEMENT DNA; | CHAIN: A, B;          |                      |                      |                        |                        |                 | YY1; CHAIN: C; ADENO-  | ASSOCIATED VIRUS P5   | INITIATOR ELEMENT DNA; |
| Table 5 | SEQ<br>FOI D   | score       |                 |                                              |                        |                    |                      |                        |                                          |                        |                       |                        |                       |                      |                      |                        |                        |                 |                        |                       |                        |                       |                      |                      |                        |                        |                 |                        |                       |                        |
| Tab     | PMF            | 200         |                 | 66.0                                         |                        |                    |                      |                        |                                          | 86.0                   |                       |                        |                       |                      |                      |                        |                        |                 | 86.0                   |                       |                        |                       |                      |                      |                        |                        |                 | 1.00                   |                       |                        |
|         | Verify         | 21026       |                 | 0.07                                         |                        |                    |                      |                        |                                          | 0.02                   |                       |                        |                       |                      |                      |                        |                        |                 | -0.00                  |                       |                        |                       |                      |                      |                        |                        |                 | 0.27                   |                       |                        |
|         | Psi            | Diasi       |                 | 4e-52                                        |                        |                    |                      |                        | ,                                        | 4e-55                  |                       |                        |                       |                      |                      |                        |                        | -               | 4e-51                  |                       |                        |                       |                      |                      |                        |                        |                 | 1.8e-49                |                       |                        |
|         | END            | ¥           |                 | 353                                          | •••                    |                    |                      |                        |                                          | 381                    |                       |                        |                       |                      |                      |                        |                        |                 | 408                    |                       |                        |                       |                      |                      |                        |                        |                 | 492                    |                       |                        |
|         | START          | <del></del> |                 | 248                                          |                        |                    |                      | •                      |                                          | 269                    |                       | •                      |                       |                      |                      |                        |                        |                 | 297                    |                       |                        |                       |                      |                      |                        |                        |                 | 382                    |                       |                        |
|         | CHAIN          | 3           |                 | O                                            |                        |                    |                      |                        |                                          | U                      |                       |                        |                       |                      |                      |                        |                        |                 | J                      |                       |                        |                       | -                    |                      |                        |                        |                 | S                      |                       |                        |
|         | PDB            |             |                 | 1ubd (                                       |                        |                    |                      |                        |                                          | 1ubd (                 |                       |                        |                       |                      |                      |                        |                        |                 | lubd                   |                       |                        |                       |                      |                      |                        |                        |                 | 1ubd                   |                       |                        |
|         | SEQ            |             |                 | 1937                                         |                        |                    |                      |                        |                                          | 1937                   |                       |                        |                       |                      |                      |                        |                        |                 | 1937                   |                       | -                      |                       |                      |                      |                        | -                      |                 | 1937                   |                       |                        |

|         | PDB annotation  | INITIATION, INITIATOR<br>ELEMENT, YY1, ZINC 2<br>FINGER PROTEIN, DNA-<br>PROTEIN RECOGNITION, 3<br>COMPLEX (TRANSCRIPTION<br>REGULATION/DNA) | COMPLEX (TRANSCRIPTION<br>REGULATION/DNA) YING-<br>YANG 1; TRANSCRIPTION<br>INITIATION, INITIATOR<br>ELEMENT, YY1, ZINC 2<br>FINGER PROTEIN, DNA-<br>PROTEIN RECOGNITION, 3<br>COMPLEX (TRANSCRIPTION<br>REGULATION/DNA) | COMPLEX (TRANSCRIPTION<br>REGULATION/DNA) YING-<br>YANG 1; TRANSCRIPTION<br>INITIATION, INITIATOR<br>ELEMENT, YY1, ZINC 2<br>FINGER PROTEIN, DNA-<br>PROTEIN RECOGNITION, 3<br>COMPLEX (TRANSCRIPTION<br>REGULATION/DNA) | COMPLEX (TRANSCRIPTION<br>REGULATION/DNA) YING-<br>YANG 1; TRANSCRIPTION<br>INITIATION, INITIATOR<br>ELEMENT, YY1, ZINC 2<br>FINGER PROTEIN, DNA-<br>PROTEIN RECOGNITION, 3 |
|---------|-----------------|----------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
|         | Compound        | CHAIN: A, B;                                                                                                                                 | YY1; CHAIN: C; ADENO-<br>ASSOCIATED VIRUS P5<br>INITIATOR ELEMENT DNA;<br>CHAIN: A, B;                                                                                                                                   | YY1; CHAIN: C; ADENO-<br>ASSOCIATED VIRUS P5<br>INITIATOR ELEMENT DNA;<br>CHAIN: A, B;                                                                                                                                   | YY1; CHAIN: C; ADENO-<br>ASSOCIATED VIRUS P5<br>INITIATOR ELEMENT DNA;<br>CHAIN: A, B;                                                                                      |
| Table 5 | SEQ<br>FOLD     |                                                                                                                                              |                                                                                                                                                                                                                          |                                                                                                                                                                                                                          |                                                                                                                                                                             |
| Tat     | PMF             |                                                                                                                                              | 1.00                                                                                                                                                                                                                     | 1.00                                                                                                                                                                                                                     | 1.00                                                                                                                                                                        |
|         | Verify<br>score |                                                                                                                                              | 80.0                                                                                                                                                                                                                     | 0.29                                                                                                                                                                                                                     | 0.10                                                                                                                                                                        |
|         | Psi<br>Blast    |                                                                                                                                              | 2e-52                                                                                                                                                                                                                    | 5.1e-34                                                                                                                                                                                                                  | 2e-56                                                                                                                                                                       |
|         | END             |                                                                                                                                              | 520                                                                                                                                                                                                                      | 548                                                                                                                                                                                                                      | 577                                                                                                                                                                         |
|         | START<br>AA     |                                                                                                                                              | 409                                                                                                                                                                                                                      | 447                                                                                                                                                                                                                      | 465                                                                                                                                                                         |
|         | CHAIN           |                                                                                                                                              | U                                                                                                                                                                                                                        | ပ                                                                                                                                                                                                                        | U                                                                                                                                                                           |
|         | PDB<br>ID       | •                                                                                                                                            | lubd                                                                                                                                                                                                                     | lubd                                                                                                                                                                                                                     | 1ubd                                                                                                                                                                        |
|         | SEQ<br>D        |                                                                                                                                              | 1937                                                                                                                                                                                                                     | 1937                                                                                                                                                                                                                     | 1937                                                                                                                                                                        |

|         | PDB annotation       | COMPLEX (TRANSCRIPTION REGULATION/DNA) | COMPLEX (TRANSCRIPTION REGULATION/DNA) YING- | YANG 1; TRANSCRIPTION  | ELEMENT. YY1. ZINC 2 | FINGER PROTEIN, DNA- | PROTEIN RECOGNITION, 3 | COMPLEX (TRANSCRIPTION | REGULATION/DNA) | COMPLEX (TRANSCRIPTION | REGULATION/DNA) YING- | YANG 1; TRANSCRIPTION  | INITIATION, INITIATOR | ELEMENT, YY1, ZINC 2 | FINGER PROTEIN, DNA- | PROTEIN RECOGNITION, 3 | COMPLEX (TRANSCRIPTION | REGULATION/DNA) | COMPLEX (TRANSCRIPTION | REGULATION/DNA) YING- | YANG 1; TRANSCRIPTION  | INITIATION, INITIATOR | ELEMENT, YY1, ZINC 2 | FINGER PROTEIN, DNA- | PROTEIN RECOGNITION, 3 | COMPLEX (TRANSCRIPTION | REGULATION/DNA) | COMPLEX (TRANSCRIPTION | REGULATION/DNA) YING- |
|---------|----------------------|----------------------------------------|----------------------------------------------|------------------------|----------------------|----------------------|------------------------|------------------------|-----------------|------------------------|-----------------------|------------------------|-----------------------|----------------------|----------------------|------------------------|------------------------|-----------------|------------------------|-----------------------|------------------------|-----------------------|----------------------|----------------------|------------------------|------------------------|-----------------|------------------------|-----------------------|
|         | Compound             |                                        | YYI; CHAIN: C; ADENO-<br>ASSOCIATED VIRUS P5 | INITIATOR ELEMENT DNA; | Chain: A, B;         |                      |                        |                        |                 | YY1; CHAIN: C; ADENO-  | ASSOCIATED VIRUS P5   | INITIATOR ELEMENT DNA; | CHAIN: A, B;          |                      |                      |                        |                        |                 | YY1; CHAIN: C; ADENO-  | ASSOCIATED VIRUS P5   | INITIATOR ELEMENT DNA; | CHAIN: A, B;          |                      |                      |                        |                        |                 | YY1; CHAIN: C; ADENO-  | ASSOCIATED VIRUS P5   |
| Table 5 | SEQ<br>FOLD<br>score |                                        |                                              |                        |                      |                      |                        |                        |                 |                        |                       |                        |                       |                      |                      |                        |                        |                 |                        |                       |                        |                       |                      |                      |                        |                        |                 | 94.34                  |                       |
| Tal     | PMF                  |                                        | 1.00                                         |                        |                      |                      |                        |                        |                 | 66.0                   |                       |                        |                       | -                    |                      |                        |                        |                 | 1.00                   |                       |                        |                       |                      |                      |                        |                        |                 |                        |                       |
|         | Verify<br>score      |                                        | 0.24                                         |                        |                      |                      |                        |                        |                 | 0.31                   |                       |                        |                       |                      |                      |                        |                        |                 | 0.22                   |                       |                        |                       |                      |                      |                        |                        |                 |                        |                       |
|         | Psi<br>Blast         |                                        | 6.8e-35                                      |                        |                      |                      |                        |                        |                 | 1e-56                  |                       |                        |                       |                      |                      |                        |                        |                 | 1.2e-54                |                       |                        |                       |                      |                      |                        |                        |                 | 1.2e-54                |                       |
|         | END                  |                                        | 604                                          |                        |                      |                      |                        |                        |                 | 632                    |                       |                        |                       |                      |                      |                        |                        |                 | 689                    |                       |                        |                       |                      |                      |                        |                        |                 | 689                    |                       |
|         | START<br>AA          |                                        | 497                                          |                        |                      |                      |                        |                        |                 | 521                    |                       |                        |                       |                      |                      |                        |                        |                 | 578                    |                       |                        |                       |                      |                      |                        |                        |                 | 579                    |                       |
|         | CHAIN                |                                        | ပ                                            |                        |                      |                      |                        |                        |                 | ၁                      |                       |                        |                       |                      |                      |                        |                        |                 | ပ                      |                       |                        |                       |                      |                      |                        |                        |                 | 2                      |                       |
|         | PDB<br>ID            |                                        | 1ubd                                         |                        |                      |                      |                        |                        |                 | 1ubd                   |                       |                        |                       |                      |                      |                        |                        |                 | 1ubd                   |                       |                        |                       |                      |                      |                        |                        |                 | 1ubd                   |                       |
|         | SEQ<br>ID<br>NO:     |                                        | 1937                                         |                        |                      |                      |                        |                        |                 | 1937                   |                       |                        |                       |                      | ,                    | •                      |                        |                 | 1937                   |                       |                        |                       | -                    |                      |                        |                        |                 | 1937                   |                       |

| Table 5   Table 5   Compound   PDB annotation                                                            |                      | COMPLEX (TRANSCRIPTION<br>REGULATION/DNA) YING-<br>YANG 1; TRANSCRIPTION<br>INTIATION, INITIATOR<br>ELEMENT, YY1, ZINC 2 | FINGER PROTEIN, DNA- |
|----------------------------------------------------------------------------------------------------------|----------------------|--------------------------------------------------------------------------------------------------------------------------|----------------------|
| Table 5  END Psi Verify PMF SEQ  AA Blast score FOLD score  745 1.2e-52 0.06 0.88  716 1.7e-34 0.35 0.99 |                      |                                                                                                                          | - 1                  |
| Hab Psi Verify PMF AA Blast score score score score 1.2e-52 0.06 0.88 745 1.7e-34 0.35 0.99              | Orenda O TAARI O AVA | YY1; CHAIN: C; ADENO-<br>ASSOCIATED VIRUS P5<br>INITIATOR ELEMENT DNA;<br>CHAIN: A, B;                                   |                      |
| END Psi Verify PM<br>AA Blast score scor<br>745 1.2e-52 0.06 0.88<br>716 1.7e-34 0.35 0.99               |                      |                                                                                                                          |                      |
| END Psi<br>AA Blast<br>745 1.2e-52 0<br>716 1.7e-34 0                                                    | 90                   | 1.00                                                                                                                     |                      |
| END<br>AA<br>745<br>716                                                                                  | 300                  | -0.05                                                                                                                    |                      |
| 72                                                                                                       | 270.25               | 3.46-35                                                                                                                  |                      |
| R A A                                                                                                    | 744                  | 444                                                                                                                      |                      |
| AA AA 605 605                                                                                            | 640                  | 040                                                                                                                      |                      |
| CHAIN ID                                                                                                 | C                    | د                                                                                                                        |                      |
| PDB<br>ID<br>1ubd                                                                                        | 1.hd                 | Dan                                                                                                                      |                      |
| SEQ<br>D<br>NO:<br>1937                                                                                  | ļ <del></del>        | 193/                                                                                                                     |                      |

|         |                 |                                               | - $-$                                  |                                              |                                                   |                      |                      |                        |                                          |                      |                                                |                        |                       |                      |                      |                        |                        |                                          |                      |                               |                       |                       |                      |                           |                             |                       |                       |
|---------|-----------------|-----------------------------------------------|----------------------------------------|----------------------------------------------|---------------------------------------------------|----------------------|----------------------|------------------------|------------------------------------------|----------------------|------------------------------------------------|------------------------|-----------------------|----------------------|----------------------|------------------------|------------------------|------------------------------------------|----------------------|-------------------------------|-----------------------|-----------------------|----------------------|---------------------------|-----------------------------|-----------------------|-----------------------|
|         | PDB annotation  | PROTEIN RECOGNITION, 3 COMPLEX (TRANSCRIPTION | REGULATION/DNA) COMPLEX (TRANSCRIPTION | REGULATION/DNA) YING-                        | I AND I; I KANSCKIP I JON<br>NITIATION, INITIATOR | ELEMENT, YY1, ZINC 2 | FINGER PROTEIN, DNA- | PROTEIN RECOGNITION, 3 | COMPLEX (IRANSCRIPTION   REGIT ATTOMORY) | COLOT FX (ME 1316)   | COMPLEX (TRANSCRIPTION   REGULATION/DNA) YING- | YANG 1; TRANSCRIPTION  | INITIATION, INITIATOR | ELEMENT, YY1, ZINC 2 | FINGER PROTEIN, DNA- | PROTEIN RECOGNITION, 3 | COMPLEX (TRANSCRIPTION | REGULATION/DNA)                          | COMPLEX (DNA-BINDING | PROTEIN/DNA) FIVE-            | FINGER GLI; GLI, ZINC | FINGER, COMPLEX (DNA- | BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING      | PROTEIN/DNA) FIVE.          | FINGER GLI; GLI, ZINC | FINGER, COMPLEX (DNA- |
|         | Compound        |                                               | YY1; CHAIN: C; ADENO-                  | ASSOCIATED VIRUS P5<br>INITIATOR ELEMENT DNA | CHAIN: A, B;                                      |                      |                      |                        |                                          | VVI: CHAIN: C. ADENO | ASSOCIATED VIRUS P5                            | INITIATOR ELEMENT DNA; | CHAIN: A, B;          |                      |                      |                        |                        | 20 C C C C C C C C C C C C C C C C C C C | CHAPIL A BAIL CITY   | Chalin: A; DINA; CHAIN: C, D; |                       |                       |                      | ZINC FINGER PROTEIN GLII; | CHAIN: A; DNA; CHAIN: C, D; |                       |                       |
| Table 5 | SEQ<br>FOLD     | 21025                                         |                                        |                                              |                                                   |                      |                      |                        |                                          |                      |                                                |                        |                       | •                    |                      | •                      |                        |                                          | •                    |                               |                       |                       |                      |                           |                             |                       | ****                  |
| Ta      | PMF             |                                               | 86.0                                   |                                              |                                                   |                      |                      |                        |                                          | 96.0                 |                                                |                        |                       |                      |                      |                        |                        | 010                                      | 0.10                 |                               |                       |                       | 5                    | 0.58                      |                             |                       |                       |
|         | Verify<br>score |                                               | 80.0                                   |                                              |                                                   |                      |                      |                        |                                          | 0.01                 |                                                |                        |                       |                      |                      |                        |                        | 20.0                                     | C7:0-                |                               |                       |                       | 0.10                 | -0.18                     |                             |                       |                       |
|         | Psi<br>Blast    |                                               | 8e-52                                  |                                              |                                                   |                      |                      |                        |                                          | 1.7e-34              |                                                |                        |                       |                      |                      |                        |                        | 1 70.73                                  | 1.70-2               |                               |                       |                       | 5 10 77              | 77-21.6                   |                             |                       |                       |
| í       | END<br>AA       |                                               | 772                                    |                                              |                                                   |                      |                      |                        |                                          | 772                  |                                                |                        |                       |                      |                      |                        |                        | 242                                      | 1                    |                               |                       |                       | 290                  | /07                       |                             |                       |                       |
| £ 4.    | SIAKI<br>AA     |                                               | 661                                    |                                              |                                                   |                      |                      |                        |                                          | 671                  |                                                |                        |                       |                      |                      |                        |                        | 114                                      | -<br>-<br>(          |                               |                       |                       | 135                  |                           |                             |                       |                       |
| CITABL  | CHAIN           |                                               | S                                      |                                              |                                                   |                      | •                    | -                      |                                          | _<br>ပ               |                                                | -                      |                       |                      |                      |                        |                        | A                                        |                      |                               |                       |                       | A                    |                           |                             |                       |                       |
| ana     | U D             |                                               | 1ubd                                   |                                              |                                                   |                      |                      |                        | 1                                        | lubd                 |                                                |                        |                       |                      |                      |                        |                        | 2gli ,                                   |                      |                               |                       |                       | 2gli /               |                           |                             |                       |                       |
| CEO     | A B B           |                                               | 1937                                   |                                              |                                                   |                      |                      |                        |                                          | 1937                 |                                                |                        |                       |                      |                      |                        |                        | 1937                                     |                      |                               |                       |                       | 1937                 |                           |                             |                       |                       |

|         | PDB annotation        | COMPLEX (DNA-BINDING<br>PROTEIN/DNA) FIVE-<br>FINGER GLI; GLI, ZINC<br>FINGER COMPLEY (DNA | BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING PROTEIN/DNA) FIVE-                  | FINGER GLI; GLI, ZINC<br>FINGER, COMPLEX (DNA- | BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING      | PROTEIN/DNA) FIVE-          | FINGER GLI, GLI, ZINC | FINGER, COMPLEX (DNA- | SOLUTION FROI EIN/DINA)   | COMPLEX (DNA-BINDING<br>PROTEIN/DNA) FIVE- | FINGER GLI; GLI, ZINC | FINGER, COMPLEX (DNA- | BINDING PROTEIN/DNA)                     | COMPLEX (DNA-BINDING        | FINGED GIT. CIT ZEIC | FINGER GLI, GLI, ZINC | FINGER, COMPLEX (DNA- | BINDING PROTEIN/DNA)       | COMPLEX (DNA-BINDING       | PROTEIN/DNA) FIVE-          | FINGER GLI; GLI, ZINC | FINGER, COMPLEX (DNA- | BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING      |
|---------|-----------------------|--------------------------------------------------------------------------------------------|----------------------|----------------------------------------------------------|------------------------------------------------|----------------------|---------------------------|-----------------------------|-----------------------|-----------------------|---------------------------|--------------------------------------------|-----------------------|-----------------------|------------------------------------------|-----------------------------|----------------------|-----------------------|-----------------------|----------------------------|----------------------------|-----------------------------|-----------------------|-----------------------|----------------------|---------------------------|
|         | Compound              | ZINC FINGER PROTEIN GLII;<br>CHAIN: A; DNA; CHAIN: C, D;                                   |                      | ZINC FINGER PROTEIN GLII;<br>CHAIN: A; DNA; CHAIN: C, D; |                                                |                      | ZINC FINGER PROTEIN GLII; | CHAIN: A; DNA; CHAIN: C, D; |                       |                       | ZNIC ENICED DE CERTE CELE | CHAIN: A; DNA; CHAIN: C, D;                |                       |                       | ייייי יייייי מייייי מייייי מייייי מייייי | CHAIN: A. DNA. CHAIN: O. D. | ( , , ) ( , , , , )  |                       |                       | ZNIC ENICED DECEMBER OF TO | CINC FINGER FROI EIN GLII; | CHAIN: A; DNA; CHAIN: C, D; |                       |                       |                      | ZINC FINGER PROTEIN GLII; |
| Table 5 | SEQ<br>FOLD           | 2008                                                                                       |                      |                                                          |                                                |                      |                           |                             |                       |                       |                           |                                            |                       | ,,,,                  |                                          |                             |                      |                       |                       |                            |                            |                             |                       | -                     |                      |                           |
| Та      | PMF<br>score          | 99.0                                                                                       |                      | 1.00                                                     |                                                |                      | 1.00                      |                             |                       |                       | 1 00                      | 7.00                                       |                       |                       | 1                                        | 1.00                        | ٠                    |                       |                       | 1 00                       | 20.1                       | •                           | -                     |                       |                      | 1.00                      |
|         | Verify<br>score       | -0.17                                                                                      |                      | -0.03                                                    |                                                |                      | 0.31                      |                             |                       |                       | 0.05                      | 9                                          |                       |                       | 0.12                                     | C1.0                        |                      |                       |                       | 0.31                       | 10.0                       |                             |                       |                       |                      | 0.50                      |
|         | Psi<br>Blast          | 2e-54                                                                                      |                      | 8e-69                                                    |                                                | ,,                   | 1.2e-66                   |                             |                       |                       | 1e-67                     | 5                                          |                       |                       | 1 20 KK                                  | 1.25-00                     |                      | -1                    |                       | 1e-69                      | \<br>}                     |                             |                       |                       | i                    | 0e-/1                     |
|         | END<br>AA             | 326                                                                                        | 7.10                 | 354                                                      | *                                              | 00,                  | 409                       | ***                         |                       |                       | 522                       |                                            |                       |                       | 550                                      |                             |                      |                       |                       | 578                        | )                          |                             |                       | •                     |                      | 900                       |
|         | START                 | 166                                                                                        | 101                  | 18/                                                      |                                                | 000                  | 7/7                       |                             |                       |                       | 356                       |                                            |                       |                       | 383                                      | }                           |                      |                       |                       | 411                        |                            | •                           |                       |                       | 167                  |                           |
|         | CHAIN                 | A                                                                                          |                      | €                                                        |                                                |                      | A                         |                             |                       |                       | A                         |                                            |                       |                       | A                                        |                             | -                    |                       |                       | A                          |                            | <del></del>                 |                       |                       |                      | 4                         |
|         | PDB                   | 2gli                                                                                       | :120                 | 1187                                                     | -                                              | :1~6                 | 1187                      |                             |                       |                       | 2gli                      | )                                          |                       |                       | 29li                                     | <br>0                       |                      |                       |                       | 2gli                       | )                          |                             |                       |                       | 2ali                 |                           |
|         | A<br>A<br>B<br>B<br>S | 1937                                                                                       | 1027                 |                                                          |                                                | 1027                 |                           |                             |                       |                       | 1937                      |                                            |                       |                       | 1937                                     |                             |                      |                       |                       | 1937                       |                            |                             |                       |                       | 1037                 | $\dashv$                  |

|         | PDB annotation       | PROTEIN/DNA) FIVE-<br>FINGER GLI; GLI, ZINC<br>FINGER, COMPLEX (DNA-<br>BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING<br>PROTEIN/DNA) FIVE-<br>FINGER GLI; GLI, ZINC<br>FINGER, COMPLEX (DNA-<br>BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING<br>PROTEIN/DNA) FIVE-<br>FINGER GLI; GLI, ZINC<br>FINGER, COMPLEX (DNA-<br>BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING<br>PROTEIN/DNA) FIVE-<br>FINGER GLI; GLI, ZINC<br>FINGER, COMPLEX (DNA-<br>BINDING PROTEIN/DNA) | COMPLEX (DNA-BINDING<br>PROTEIN/DNA) FIVE-<br>FINGER GLI; GLI, ZINC<br>FINGER, COMPLEX (DNA-<br>BINDING PROTEIN/DNA) | GLYCOPROTEIN MEMBRANE COFACTOR PROTEIN (MCP); VIRUS RECEPTOR, COMPLEMENT COFACTOR, SHORT CONSENSUS REPEAT, 2 SCR, |
|---------|----------------------|----------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------|
|         | Compound             | CHAIN: A; DNA; CHAIN: C, D;                                                                  | ZINC FINGER PROTEIN GL11;<br>CHAIN: A; DNA; CHAIN: C, D;                                                             | ZINC FINGER PROTEIN GL11;<br>CHAIN: A; DNA; CHAIN: C, D;                                                             | ZINC FINGER PROTEIN GL11;<br>CHAIN: A; DNA; CHAIN: C, D;                                                             | ZINC FINGER PROTEIN GL11;<br>CHAIN: A; DNA; CHAIN: C, D;                                                             | CD46; CHAIN: A, B, C, D, E, F;                                                                                    |
| Table 5 | SEQ<br>FOLD<br>score |                                                                                              | 19.96                                                                                                                |                                                                                                                      |                                                                                                                      |                                                                                                                      |                                                                                                                   |
| Tał     | PMF                  |                                                                                              |                                                                                                                      | 1.00                                                                                                                 | 96.0                                                                                                                 | 0.86                                                                                                                 | 0.84                                                                                                              |
|         | Verify<br>score      |                                                                                              |                                                                                                                      | 0.44                                                                                                                 | 0.13                                                                                                                 | 0.26                                                                                                                 | 0.76                                                                                                              |
|         | Psi<br>Blast         |                                                                                              | 6e-71                                                                                                                | 6e-70                                                                                                                | 6e-70                                                                                                                | 6.8e-34                                                                                                              | 1.2e-10                                                                                                           |
|         | END                  |                                                                                              | 662                                                                                                                  | 069                                                                                                                  | 774                                                                                                                  | 771                                                                                                                  | 321                                                                                                               |
|         | START<br>AA          |                                                                                              | 523                                                                                                                  | 551                                                                                                                  | 209                                                                                                                  | 643                                                                                                                  | 264                                                                                                               |
|         | CHAIN                |                                                                                              | A                                                                                                                    | A                                                                                                                    | A                                                                                                                    | A                                                                                                                    | A                                                                                                                 |
| •       | PDB<br>ID            |                                                                                              | 2gli                                                                                                                 | 2gli                                                                                                                 | 2gli                                                                                                                 | 2gli                                                                                                                 | lcki                                                                                                              |

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| 1938   1-55g   A   26-46   371   51-5-11   0.644   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00   1.00  |       |                      |                                |                                |                   |                      |                |                          |                |              |                       |                             |                              |                                |                              |          |               |            |                  |         |                      |                        | —                     |                     |       |                      |                         |                       |       | 1 |
|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------|----------------------|--------------------------------|--------------------------------|-------------------|----------------------|----------------|--------------------------|----------------|--------------|-----------------------|-----------------------------|------------------------------|--------------------------------|------------------------------|----------|---------------|------------|------------------|---------|----------------------|------------------------|-----------------------|---------------------|-------|----------------------|-------------------------|-----------------------|-------|---|
| Table 5   Table 5   Table 5   Table 5   Table 5   Table 5   Table 6   Table 6   Table 6   Table 6   Table 7   Table 8   Tabl |       | PDB annotation       | MEASLES VIRUS,<br>GLYCOPROTEIN | GLYCOPROTEIN                   | MEMBRANE COFACTOR | PROTEIN (MCP); VIRUS | COFACTOR SHORT | CONSENSUS REPEAT, 2 SCR, | MEASLES VIRUS, | GLYCOPROTEIN | SERINE PROTEINASE     | COAGULATION FACTOR II;      | EFTOMODIE IN TW CD141        | ANTIGEN; EGR-CMK SERINE        | PROTEINASE, EGF-LIKE         | DOMAINS, | ANTICOAGULANT | COMPLEX, 2 | ANTIFIBRINOLYTIC | COMPLEX | COMPLEMENT INHIBITOR | VCP, SP35; COMPLEMENT, | NMK, MODULES, PROTEIN | STRUCTURE, VACCINIA | VIRUS | COMPLEMENT INHIBITOR | VCF, SF33; COMFLEMEN I, | NMR, MODULES, PROTEIN | VIRUS |   |
| PDB                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |       | Compound             |                                | CD46; CHAIN: A, B, C, D, E, F; |                   |                      |                |                          |                |              | THROMBIN LIGHT CHAIN; | CHAIN: A, B, C, D; THROMBIN | D. TUDOMEDOMONIII DI. CHADI. | I, J. K. L. THROMBIN INHIBITOR | L-GLÚ-L-GLY-L-ARM; CHAIN: E, | F, G, H; |               |            |                  |         | COMPLEMENT CONTROL   | PROTEIN; CHAIN: A;     |                       |                     |       | COMPLEMENT CONTROL   | PKOLEIN; CHAIN: A;      |                       |       |   |
| PDB                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          | ble 5 | SEQ<br>FOLD<br>score |                                |                                |                   |                      |                |                          |                |              |                       |                             |                              |                                |                              |          |               |            |                  |         |                      |                        |                       |                     |       |                      |                         |                       |       |   |
| PDB   CHAIN   START   END   Psi                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | Ta    | PMF                  |                                | 0.95                           |                   |                      |                |                          |                |              | -0.19                 |                             |                              |                                |                              |          |               |            |                  |         | 1.00                 |                        |                       |                     |       | -0.19                |                         |                       |       |   |
| PDB   CHAIN   START   END                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |       | Verify<br>score      | -                              | 0.59                           |                   |                      |                |                          |                |              | 0.25                  |                             |                              |                                |                              |          |               |            |                  |         | 0.64                 |                        |                       |                     |       | 0.03                 |                         |                       |       |   |
| PDB   CHAIN   START                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |       | Psi<br>Blast         |                                | 2.4e-10                        |                   |                      |                |                          |                |              | 1.7e-12               |                             |                              |                                |                              |          |               |            |                  |         | 5.1e-11              |                        |                       |                     |       | 1.5e-09              |                         |                       |       |   |
| PDB CHAIN D D 1ckl A 6 1dx5 I 6 1e5g A 7                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |       | END<br>AA            |                                | 117                            |                   |                      |                |                          |                |              | 173                   |                             |                              |                                |                              |          |               |            |                  |         | 371                  |                        |                       |                     |       | 113                  |                         |                       |       |   |
| PDB                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |       | START<br>AA          |                                | 61                             |                   |                      |                |                          |                |              | 55                    |                             |                              |                                |                              |          |               |            |                  |         | 264                  |                        |                       | -                   |       | 3                    |                         |                       |       |   |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |       | CHAIN                |                                | A                              |                   |                      |                |                          |                |              | I                     |                             |                              |                                |                              |          |               |            |                  |         | A                    |                        |                       |                     |       | A                    |                         |                       |       |   |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |       | PDB<br>ID            |                                | 1ck1                           |                   |                      |                |                          |                |              | 1dx5                  |                             |                              |                                |                              |          |               |            |                  |         | 1e5g                 | )                      |                       |                     |       | 1e5g                 |                         |                       |       |   |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |       | SEQ<br>ID<br>NO:     |                                | $\vdash$                       |                   |                      |                |                          |                |              | 1938                  |                             |                              |                                |                              |          |               |            |                  |         | 1938                 |                        |                       |                     |       | 1938                 |                         |                       |       |   |

|         | PDB annotation       | COMPLEMENT INHIBITOR VCP, SP35; COMPLEMENT, NMR, MODULES, PROTEIN STRUCTURE, VACCINIA VIRUS | MATRIX PROTEIN EXTRACELLULAR MATRIX, CALCIUM-BINDING, GLYCOPROTEIN, 2 REPEAT, SIGNAL, MULTIGENE FAMILY, DISEASE MUTATION, 3 EGF-LIKE DOMAIN, HUMAN FIBRILLIN-1 FRAGMENT, MATRIX PROTEIN | MATRIX PROTEIN EXTRACELLULAR MATRIX, CALCIUM-BINDING, GLYCOPROTEIN, 2 REPEAT, SIGNAL, MULTIGENE FAMILY, DISEASE MUTATION, 3 EGF-LIKE DOMAIN, HUMAN FIBRILLIN-1 FRAGMENT, MATRIX PROTEIN | BLOOD CLOTTING PROTEIN INHIBITOR COMPLEX, COAGULATION COFACTOR, PROTEASE |                                         |
|---------|----------------------|---------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------|-----------------------------------------|
|         | Compound             | COMPLEMENT CONTROL<br>PROTEIN; CHAIN: A;                                                    | FIBRILLIN; CHAIN: NULL;                                                                                                                                                                 | FIBRILLIN; CHAIN: NULL;                                                                                                                                                                 | COAGULATION FACTOR XA;<br>CHAIN: A; COAGULATION<br>FACTOR XA; CHAIN: L;  | GLYCOPROTEIN 16TH<br>COMPLEMENT CONTROL |
| Table 5 | SEQ<br>FOLD<br>score |                                                                                             |                                                                                                                                                                                         |                                                                                                                                                                                         |                                                                          |                                         |
| Ta      | PMF<br>score         | -0.18                                                                                       | -0.20                                                                                                                                                                                   | -0.17                                                                                                                                                                                   | 0.03                                                                     | 0.88                                    |
|         | Verify<br>score      | 0.21                                                                                        | 0.07                                                                                                                                                                                    | 0.05                                                                                                                                                                                    | -0.01                                                                    | 0.63                                    |
|         | Psi<br>Blast         | 1.2e-11                                                                                     | 5.1e-12                                                                                                                                                                                 | 6.8e-09                                                                                                                                                                                 | 3.4e-06                                                                  | 8.4e-11                                 |
|         | END<br>AA            | 186                                                                                         | 247                                                                                                                                                                                     | 338                                                                                                                                                                                     | 108                                                                      | 321                                     |
|         | START                | 61                                                                                          | 176                                                                                                                                                                                     | 257                                                                                                                                                                                     | 65                                                                       | 263                                     |
|         | CHAIN<br>ID          | A                                                                                           |                                                                                                                                                                                         |                                                                                                                                                                                         | <b>⊢</b>                                                                 |                                         |
|         | PDB<br>ID            | 1e5g                                                                                        | lemn                                                                                                                                                                                    | lemn                                                                                                                                                                                    | 1fjs                                                                     | 1hcc                                    |

| _       |                      |                                        |                                                                                   |                                                      |                                 |                       |                              |                   |                 |                |               |                       |                  |                           |                 |                |                    |               |                       |                  |                     |
|---------|----------------------|----------------------------------------|-----------------------------------------------------------------------------------|------------------------------------------------------|---------------------------------|-----------------------|------------------------------|-------------------|-----------------|----------------|---------------|-----------------------|------------------|---------------------------|-----------------|----------------|--------------------|---------------|-----------------------|------------------|---------------------|
|         | PDB annotation       |                                        |                                                                                   | MEMBRANE ADHESION<br>SHORT CONSENSUS<br>REPFAT SUSHI | COMPLEMENT CONTROL PROTFIN 2 N- | GLYCOSYLATION, MULTI- | DOMAIN, MEMBRANE<br>ADHESION | MEMBRANE ADHESION | SHORT CONSENSUS | REPEAT, SUSHI, | PROTEIN, 2 N- | GLYCOSYLATION, MULTI- | DOMAIN, MEMBRANE | MEMBRANE ADHESTON         | SHORT CONSENSUS | REPEAT, SUSHI, | COMPLEMENT CONTROL | PROTEIN, 2 N- | GLYCOSYLATION, MULTI- | DOMAIN, MEMBRANE | SPERMADHESIN ACIDIC |
|         | Compound             | PROTEIN (/CCP\$) OF FACTOR H<br>1HCC 3 | GLYCOPROTEIN 16TH<br>COMPLEMENT CONTROL<br>PROTEIN (/CCP\$) OF FACTOR H<br>1HCC 3 | I BETA2-GLYCOPROTEIN<br>I: A;                        |                                 |                       |                              | 'A2-GLYCOPROTEIN  | I; CHAIN: A;    |                |               |                       |                  | HIMAN BETA2-GI VCOPROTEIN | I; CHAIN: A;    |                |                    |               |                       |                  | ASFP; CHAIN: NULL;  |
| Table 5 | SEQ<br>FOLD<br>score |                                        |                                                                                   |                                                      |                                 |                       |                              | 94.07             |                 |                |               |                       |                  |                           |                 |                |                    |               |                       |                  |                     |
| Tak     | PMF                  |                                        | 0.18                                                                              | -0.06                                                |                                 |                       |                              |                   |                 |                |               |                       |                  | -0.10                     |                 |                |                    |               |                       |                  | 0.24                |
|         | Verify<br>score      |                                        | 0.52                                                                              | 0.37                                                 |                                 |                       |                              |                   |                 |                |               |                       |                  | 0.13                      | 0.10            |                |                    |               |                       |                  | 0.55                |
|         | Psi<br>Blast         |                                        | 3.6e-10                                                                           | 3.4e-09                                              |                                 |                       |                              | 5.1e-24           |                 |                |               |                       |                  | 5 10 21                   | 7.10-21         |                |                    |               |                       |                  | 2.4e-27             |
|         | END                  |                                        | 118                                                                               | 377                                                  |                                 |                       |                              | 393               |                 |                |               |                       |                  | 255                       | 000             |                |                    |               |                       |                  | 260                 |
|         | START<br>AA          |                                        | 09                                                                                | 239                                                  |                                 |                       |                              | 58                |                 |                |               |                       |                  | 77                        | <b>T</b>        |                |                    |               |                       |                  | 125                 |
|         | CHAIN<br>ID          |                                        |                                                                                   | A                                                    |                                 |                       |                              | A                 |                 |                |               |                       |                  | <                         | ť               |                |                    |               |                       |                  |                     |
|         | PDB<br>ID            |                                        | 1hcc                                                                              | 1qub                                                 |                                 |                       |                              | 1qub              | 1               |                |               |                       |                  | 10.1                      | anhı            |                |                    |               |                       |                  | 1sfp                |
|         | SEQ<br>EQ            |                                        | 1938                                                                              | 1938                                                 |                                 |                       |                              | 1938              |                 |                |               |                       |                  | 1070                      | 1930            |                |                    |               |                       |                  | 1938                |

|         | PDB annotation       | SEMINAL PROTEIN;<br>SPERMADHESIN, BOVINE<br>SEMINAL PLASMA | SEMINAL FLUID PROTEIN, | ASFF, CUB DOMAIN, X-KAY<br>CRYSTAL 3 STRUCTURE,<br>GROWTH FACTOR | SPERMADHESIN ACIDIC SEMINAL PROTEIN; | SPERMADHESIN, BOVINE | PROTEIN, ACIDIC 2 | SEMINAL FLUID PROTEIN, | ASFP, CUB DOMAIN, X-RAY CRYSTAL 3 STRUCTURE. | GROWTH FACTOR | COMPLEX (SEMINAL PLASMA PROTEIN/SPP)               | SEMINAL PLASMA<br>PROTEINS                          | SPERMADHESINS, CUB | DOMAIN 2 ARCHITECTURE, | COMPLEX (SEMINAL | PLASMA PROTEIN/SPP) | COMPLEX (SEMINAL  PI A SMA PROTFIN/SPP)           | SEMINAL PLASMA          | PROTEINS,                   | SPERMADHESINS, CUB<br>DOMAIN 2 ARCHITECTURE, |
|---------|----------------------|------------------------------------------------------------|------------------------|------------------------------------------------------------------|--------------------------------------|----------------------|-------------------|------------------------|----------------------------------------------|---------------|----------------------------------------------------|-----------------------------------------------------|--------------------|------------------------|------------------|---------------------|---------------------------------------------------|-------------------------|-----------------------------|----------------------------------------------|
|         | Compound             |                                                            |                        |                                                                  | ASFP; CHAIN: NULL;                   |                      |                   |                        |                                              |               | MAJOR SEMINAL PLASMA<br>GLYCOPROTEIN PSP-I; CHAIN: | A; MAJOR SEMINAL PLASMA GLYCOPROTEIN PSP-II: CHAIN: | В                  |                        |                  |                     | MAJOR SEMINAL PLASMA GI VCOPPOTEIN POP. I. CHAIN: | A: MAJOR SEMINAL PLASMA | GLYCOPROTEIN PSP-II; CHAIN: | В                                            |
| Table 5 | SEQ<br>FOLD<br>score |                                                            |                        |                                                                  |                                      |                      |                   |                        |                                              |               |                                                    |                                                     |                    |                        |                  |                     |                                                   |                         |                             |                                              |
| Tal     | PMF<br>score         |                                                            |                        |                                                                  | 0.01                                 |                      |                   |                        |                                              |               | 90.0                                               |                                                     |                    |                        |                  |                     | 0.17                                              |                         |                             |                                              |
|         | Verify<br>score      | as a                                                       |                        |                                                                  | -0.22                                |                      |                   |                        |                                              |               | 0.42                                               |                                                     |                    |                        |                  |                     | -0.06                                             |                         |                             |                                              |
|         | Psi<br>Blast         |                                                            |                        |                                                                  | 7.2e-09                              |                      |                   |                        |                                              |               | 1.2e-27                                            |                                                     |                    |                        |                  |                     | 6e-12                                             |                         |                             |                                              |
|         | END<br>AA            |                                                            |                        |                                                                  | 411                                  |                      |                   |                        |                                              |               | 261                                                |                                                     |                    |                        |                  |                     | 411                                               |                         |                             |                                              |
|         | START<br>AA          |                                                            |                        |                                                                  | 323                                  |                      |                   |                        |                                              |               | 127                                                |                                                     |                    |                        |                  |                     | 325                                               |                         |                             |                                              |
|         | CHAIN<br>ID          |                                                            |                        |                                                                  |                                      |                      |                   |                        |                                              | _             | A                                                  |                                                     |                    |                        |                  |                     | Ą                                                 |                         |                             |                                              |
|         | PDB<br>ID            |                                                            |                        | M2-010-0-0                                                       | 1sfp                                 |                      |                   |                        |                                              | ٠             | 1spp                                               |                                                     |                    |                        |                  |                     | 1spp                                              |                         |                             |                                              |
|         | SEQ<br>D<br>NO:      |                                                            |                        |                                                                  | 1938                                 |                      |                   |                        |                                              |               | 1938                                               |                                                     |                    |                        |                  |                     | 1938                                              |                         |                             |                                              |

| ,       | PDB annotation  |       | COMPLEX (SEMINAL | FLASIMA FROI EIN/SFF) | COMPLEMENT INHIBITOR | SF35, VCF, VACCINIA VIKUS | SP35; COMPLEMENT      | MODITE SON STIER | MODOLE, SCK, SUSHI<br>DOMAIN, 2 MODULE PAIR | COMPLEMENT INHIBITOR | SP35, VCP, VACCINIA VIRUS | SP35; COMPLEMENT      | INHIBITOR, COMPLEMENT | MODULE, SCR, SUSHI | DOMAIN, 2 MODULE PAIR | COMPLEMENT INHIBITOR | SP35, VCP, VACCINIA VIRUS | SP35; COMPLEMENT      | INHIBITOR, COMPLEMENT | MODULE, SCR, SUSHI | DOMAIN, 2 MODULE PAIR | COMPLEMENT INHIBITOR | SP35, VCP, VACCINIA VIRUS | SP35; COMPLEMENT      | INHIBITOR, COMPLEMENT | MODULE, SCR, SUSHI | DOMAIN, 2 MODULE PAIR | BLOOD COAGULATION        | FACTOR STUART FACTOR; | BLOOD COAGULATION | FACTOR, SERINE | PROTEINASE, EPIDERMAL 2 |
|---------|-----------------|-------|------------------|-----------------------|----------------------|---------------------------|-----------------------|------------------|---------------------------------------------|----------------------|---------------------------|-----------------------|-----------------------|--------------------|-----------------------|----------------------|---------------------------|-----------------------|-----------------------|--------------------|-----------------------|----------------------|---------------------------|-----------------------|-----------------------|--------------------|-----------------------|--------------------------|-----------------------|-------------------|----------------|-------------------------|
|         | Compound        |       |                  | CARACTA TALESCO TALE  | VACCINIA VIRUS       | DEOTERI, CITARI MILLI     | PROTEIN; CHAIN: NOLL; |                  |                                             | VACCINIA VIRUS       | COMPLEMENT CONTROL        | PROTEIN; CHAIN: NULL; |                       |                    |                       | VACCINIA VIRUS       | COMPLEMENT CONTROL        | PROTEIN; CHAIN: NULL; |                       |                    |                       | VACCINIA VIRUS       | COMPLEMENT CONTROL        | PROTEIN; CHAIN: NULL; |                       |                    |                       | BLOOD COAGULATION FACTOR | XA; CHAIN: L, C;      |                   |                |                         |
| Table 5 | SEQ<br>FOLD     | score |                  |                       |                      |                           |                       |                  |                                             |                      |                           |                       |                       |                    |                       |                      |                           |                       |                       |                    |                       |                      |                           |                       |                       |                    |                       |                          |                       |                   |                |                         |
| Ta      | PMF             |       |                  | 7,0                   | 65.0                 |                           |                       |                  |                                             | 0.39                 |                           |                       |                       |                    |                       | 0.13                 |                           |                       |                       |                    |                       | -0.12                |                           |                       |                       |                    |                       | -0.18                    |                       |                   |                |                         |
|         | Verify<br>score |       |                  | 110                   | 0.3/                 |                           |                       |                  |                                             | 0.34                 |                           |                       |                       |                    |                       | 0.30                 |                           |                       |                       |                    |                       | 0.23                 |                           |                       |                       |                    |                       | 0.19                     |                       |                   |                |                         |
|         | Psi<br>Blast    |       |                  | 1 7- 00               | 1./e-09              |                           |                       |                  |                                             | 2.4e-13              |                           |                       |                       |                    |                       | 2.4e-10              |                           |                       |                       |                    |                       | 3.4e-10              |                           |                       |                       |                    |                       | 1.4e-08                  |                       |                   |                |                         |
|         | END             |       |                  | הרר                   | 2//                  |                           |                       |                  |                                             | 353                  |                           |                       |                       |                    |                       | 153                  |                           |                       |                       |                    |                       | 186                  |                           |                       |                       |                    |                       | 147                      |                       |                   |                |                         |
|         | START<br>AA     |       |                  | 196                   | 707                  |                           |                       |                  |                                             | 264                  |                           |                       |                       |                    |                       | 61                   |                           |                       |                       |                    |                       | 61                   |                           |                       |                       |                    |                       | 09                       |                       |                   |                |                         |
|         | CHAIN<br>ID     |       |                  |                       |                      |                           |                       |                  |                                             |                      |                           |                       |                       |                    |                       |                      |                           | _                     |                       |                    |                       |                      |                           |                       |                       |                    |                       | ì                        |                       |                   |                |                         |
|         | PDB<br>ID       |       |                  | 1                     | 1 0 0 0              |                           |                       |                  |                                             | lvvc                 |                           |                       |                       |                    |                       | lvvc                 |                           | •                     |                       |                    |                       | lvvc                 |                           |                       |                       |                    | ,                     | lxka                     | _                     |                   |                |                         |
|         | S<br>E<br>E     | :SC:  |                  | 1020                  | 1930                 |                           | į                     |                  |                                             | 1938                 |                           | 1.00                  |                       |                    |                       | 1938                 |                           |                       |                       |                    | 000                   | 1938                 |                           |                       |                       |                    |                       | 1938                     |                       |                   |                |                         |

|         |                |        |                           | _    |                                                                                                                                  |              |                                         |                                        |                                         |                                        |                        |                                                 |                       |                | _                      |                            |                           |                        |                          |                            |
|---------|----------------|--------|---------------------------|------|----------------------------------------------------------------------------------------------------------------------------------|--------------|-----------------------------------------|----------------------------------------|-----------------------------------------|----------------------------------------|------------------------|-------------------------------------------------|-----------------------|----------------|------------------------|----------------------------|---------------------------|------------------------|--------------------------|----------------------------|
| Table 5 | PDB annotation |        | GROWTH FACTOR LIKE DOMAIN |      | GLYCOPROTEIN MEMBRANE COFACTOR PROTEIN (MCP); VIRUS RECEPTOR, COMPLEMENT COFACTOR, SHORT CONSENSUS REPEAT, 2 SCR, MEASTER VIDERS | GLYCOPROTEIN |                                         |                                        |                                         |                                        |                        |                                                 |                       |                |                        |                            |                           |                        |                          |                            |
|         | Compound       |        |                           |      | CD46; CHAIN: A, B, C, D, E, F;                                                                                                   |              | GLYCOPROTEIN 16TH<br>COMPLEMENT CONTROL | PROTEIN (/CCP\$) OF FACTOR H<br>1HCC 3 | GLYCOPROTEIN 16TH<br>COMPLEMENT CONTROL | PROTEIN (/CCP\$) OF FACTOR H<br>IHCC 3 | GLYCOPROTEIN FACTOR H, | 15TH AND 16TH C-MODULE PAR (NAP MENTATED THEFT) | 1 AVERAGED STRUCTURE) | 1HFH 4 1HFHA 5 | GLYCOPROTEIN FACTOR H, | MINIMIZED AVERAGED 1HFIA 1 | STRUCTURE) 1HFI 4 1HFIA 5 | GLYCOPROTEIN FACTOR H, | 15TH C-MODULE PAIR (NMR, | MINIMIZED AVERAGED 1HFIA 1 |
|         | SEQ            | FOLD   |                           |      | 50.88                                                                                                                            |              |                                         |                                        |                                         |                                        |                        |                                                 |                       |                |                        |                            |                           |                        |                          |                            |
| Ta      | PMF            | score  |                           |      |                                                                                                                                  |              | 0.82                                    |                                        | 0.88                                    |                                        | 0.98                   |                                                 |                       |                | 0.99                   | -                          |                           | 0.89                   |                          |                            |
|         | Verify         | score  |                           |      |                                                                                                                                  |              | 0.91                                    |                                        | 0.63                                    |                                        | 96.0                   |                                                 |                       |                | 68.0                   |                            |                           | 0.42                   |                          |                            |
|         | Psi            | Blast  |                           | 0    | 1.2e-22                                                                                                                          |              | 6e-11                                   |                                        | 8.5e-09                                 |                                        | 6e-10                  | -                                               |                       |                | 1.7e-09                |                            |                           | 8e-11                  |                          |                            |
|         |                | AA     |                           | Ę    | 173                                                                                                                              |              | 170                                     |                                        | 170                                     |                                        | 175                    |                                                 |                       |                | 171                    |                            |                           | 170                    |                          |                            |
|         | START          | AA     |                           | 40   | 46<br>0                                                                                                                          |              | 112                                     |                                        | 113                                     |                                        | 112                    |                                                 |                       |                | 109                    |                            |                           | 112                    |                          |                            |
|         | CHAIN          | 3      |                           | ~    | ∢                                                                                                                                |              |                                         |                                        |                                         |                                        |                        |                                                 |                       |                |                        |                            |                           |                        |                          |                            |
| 4       | PUB            | }      |                           | 1011 | ICKI                                                                                                                             | ;            | Incc                                    |                                        | Thcc                                    |                                        | lhth                   |                                                 | -                     | ;              | Infi                   |                            | į.                        | HHI                    |                          |                            |
| One     | ) E            | N<br>Ö |                           | 1020 | 1939                                                                                                                             | 9            | 1939                                    | 9                                      | 1939                                    |                                        | 1939                   |                                                 |                       | 0001           | 1939                   |                            | 0001                      | 1939                   |                          |                            |

|         | _               |          |                           |                      |                           |                       |                       |                    |                       | <del></del>          |                           |                       |                       |                    |                       | _, |
|---------|-----------------|----------|---------------------------|----------------------|---------------------------|-----------------------|-----------------------|--------------------|-----------------------|----------------------|---------------------------|-----------------------|-----------------------|--------------------|-----------------------|----|
|         | PDB annotation  |          |                           | COMPLEMENT INHIBITOR | SP35, VCP, VACCINIA VIRUS | SP35; COMPLEMENT      | INHIBITOR, COMPLEMENT | MODULE, SCR, SUSHI | DOMAIN, 2 MODULE PAIR | COMPLEMENT INHIBITOR | SP35, VCP, VACCINIA VIRUS | SP35; COMPLEMENT      | INHIBITOR, COMPLEMENT | MODULE, SCR, SUSHI | DOMAIN, 2 MODULE PAIR |    |
|         | Compound        | •        | STRIICTIRE) 1HF14 1HF14 5 | VACCINIA VIRUS       | COMPLEMENT CONTROL        | PROTEIN; CHAIN: NULL; |                       |                    |                       | VACCINIA VIRUS       | COMPLEMENT CONTROL        | PROTEIN; CHAIN: NULL; |                       |                    |                       |    |
| Table 5 | SEQ             | FOLD     |                           |                      |                           |                       |                       |                    |                       |                      |                           |                       |                       |                    |                       |    |
| Ľ       | PMF             | score    |                           | 0.46                 |                           |                       |                       |                    |                       | -0.14                |                           |                       |                       |                    |                       |    |
|         | Verify          | score    |                           | 0.91                 |                           |                       |                       |                    |                       | 0.31                 |                           |                       |                       |                    |                       |    |
|         | Psi             | Blast    |                           | 2e-10                |                           |                       |                       |                    |                       | 6.8e-26 0.31         |                           |                       |                       |                    |                       |    |
|         | END             | AA       |                           | 176                  |                           |                       |                       |                    |                       | 171                  |                           |                       |                       |                    |                       |    |
|         | START           | AA       |                           | 113                  |                           |                       |                       |                    |                       | 53                   |                           |                       |                       |                    |                       |    |
| i       | CHAIN START END |          |                           |                      |                           |                       |                       |                    |                       |                      |                           |                       |                       | •                  |                       |    |
| ĺ       | PDB             | ON ON ON |                           | lvvc                 |                           |                       |                       |                    |                       | Iwc                  |                           |                       |                       |                    |                       |    |
|         | SEQ             | NO E     |                           | 1939                 |                           |                       |                       |                    |                       | 9561                 |                           |                       |                       |                    |                       |    |
|         |                 |          |                           |                      |                           |                       |                       |                    |                       |                      |                           |                       |                       |                    |                       |    |

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Table 6

| SEQ ID NO:     | SEQ ID NO:     | SEQ ID NO: | SEQ ID NO: | Identification of                       |
|----------------|----------------|------------|------------|-----------------------------------------|
| of full-length | of full-length | of contig  | of contig  | Priority Application                    |
| nucleotide     | peptide        | nucleotide | peptide    | that contig<br>nucleotide sequence      |
| sequence       | sequence       | sequence   | sequence   | was filed (Attorney                     |
|                |                |            |            | Docket No. SEQ ID                       |
|                |                |            |            | NO.) *                                  |
|                | -              |            |            | 110.)                                   |
| 1              | 972            | 1943       | 2710       | 784 1224                                |
| 2              | 973            | 15-15      | 2710       | , , , , , , , , , , , , , , , , , , , , |
| 3              | 974            |            |            |                                         |
| 4              | 975            |            |            |                                         |
| 5              | 976            | 1944       | 2711       | 784 852                                 |
| 6              | 977            | 1945       | 2712       | 787 7208                                |
| 7              | 978            | 1946       | 2713       | 784 7010                                |
| 8              | 979            | 1947       | 2714       | 784 3474                                |
| 9              | 980            | 1948       | 2715       | 784 3474                                |
| 10             | 981            | 1949       | 2716       | 784 8297                                |
| 11             | 982            | 1950       | 2717       | 784 7231                                |
| 12             | 983            | 1951       | 2718       | 784 8635                                |
| 13             | 984            | 1952       | 2719       | 790 1453                                |
| 14             | 985            | 1953       | 2720       | 784 9466                                |
| 15             | 986            | 1954       | 2721       | 787 1547                                |
| 16             | 987            | 1955       | 2722       | 784 1853                                |
| 17             | 988            | 1956       | 2723       | 784 5326                                |
| 18             | 989            | 1957       | 2724       | 784 3005                                |
| 19             | 990            | 1958       | 2725       | 790 10069                               |
| 20             | 991            | 1959       | 2726       | 784 2125                                |
| 21             | 992            | 1960       | 2727       | 790 19500                               |
| 22             | 993            | 1961       | 2728       | 784 1517                                |
| 23             | 994            | 1962       | 2729       | 784 2106                                |
| 24             | 995            | 1963       | 2730       | 789 2757                                |
| 25             | 996            | 1964       | 2731       | 791 2477                                |
| 26             | 997            | 1965       | 2732       | 784 6204                                |
| 27             | 998            |            |            |                                         |
| 28             | 999            | 1966       | 2733       | 784 5039                                |
| 29             | 1000           | 1967       | 2734       | 790 9623                                |
| 30             | 1001           | 1968       | 2735       | 784 6161                                |
| 31             | 1002           | 1969       | 2736       | 784_3807                                |
| 32             | 1003           |            |            |                                         |
| 33             | 1004           | 1970       | 2737       | 785_2867                                |
| 34             | 1005           | 1971       | 2738       | 784_1004                                |
| 35             | 1006           | 1972       | 2739       | 784_1004                                |
| 36             | 1007           | 1973       | 2740       | 784_6766                                |
| 37             | 1008           | 1974       | 2741       | 787_5068                                |
| 38             | 1009           | 1975       | 2742       | 788_13638                               |
| 39             | 1010           |            |            |                                         |
| 40             | 1011           | 1976       | 2743       | 784_7484                                |
| 41             | 1012           | 1977       | 2744       | 788_4366                                |
| 42             | 1013           | 1978       | 2745       | 787_3314                                |
| 43             | 1014           | 1979       | 2746       | 784_5215                                |
| 44             | 1015           | 1980       | 2747       | 784_4678                                |
| 45             | 1016           | 1981       | 2748       | 788_12744                               |
| 46             | 1017           | 1982       | 2749       | 788_12744                               |
| 47             | 1018           | 1983       | 2750       | 789_2737                                |
| 48             | 1019           | 1984       | 2751       | 790_20069                               |

1128

Table 6

| SEQ ID NO:     | SEQ ID NO:     | SEQ ID NO:   | SEQ ID NO:   | Identification of    |
|----------------|----------------|--------------|--------------|----------------------|
| of full-length | of full-length | of contig    | of contig    | Priority Application |
| nucleotide     | peptide        | nucleotide   | peptide      | that contig          |
| sequence       | sequence       | sequence     | sequence     | nucleotide sequence  |
|                |                |              |              | was filed (Attorney  |
|                |                |              |              | Docket NoSEQ ID      |
|                | 1000           | 1005         | 0750         | NO.) *               |
| 49             | 1020           | 1985         | 2752         |                      |
| 50             | 1021           | 1986         | 2753<br>2754 | 784_9000<br>784_5280 |
| 51             | 1022           | 1987         | 2755         | 789 6142             |
| 52             | 1023           | 1988<br>1989 | 2756         | 788 7211             |
| 53             | 1024<br>1025   | 1990         | 2757         | 784 897              |
| 54             |                | 1990         | 2758         | 784 4500             |
| 55<br>56       | 1026<br>1027   | 1991         | 2759         | 788 13656            |
| 57             | 1028           | 1992         | 2760         | 788_13656            |
| 58             | 1029           | 1993         | 2761         | 784 3451             |
| 59             |                | 1994         | 2762         | 792 2255             |
| 60             | 1030<br>1031   | 1996         | 2762         | 788 4373             |
| 61             | 1031           | 1997         | 2764         | 785 3219             |
| 62             | 1032           | 1998         | 2765         | 790 4641             |
| 63             | 1034           | 1990         | 2703         | 170_7071             |
| 64             | 1034           | 1999         | 2766         | 784 10172            |
| 65             | 1036           | 2000         | 2767         | 789 5937             |
| 66             | 1030           | 2001         | 2768         | 784 7576             |
| 67             | 1037           | 2001         | 2700         | 764_7370             |
| 68             | 1039           | 2002         | 2769         | 784 4621             |
| 69             | 1040           | 2003         | 2770         | 784 4621             |
| 70             | 1040           | 2004         | 2771         | 789 6210             |
| 71             | 1042           | 2005         | 2772         | 784 149              |
| 72             | 1043           | 2006         | 2773         | 789 5115             |
| 73             | 1044           | 2007         | 2774         | 789 5115             |
| 74             | 1045           | 2008         | 2775         | 789 5115             |
| 75             | 1046           | 2009         | 2776         | 784 4288             |
| 76             | 1047           | 2010         | 2777         | 790 19387            |
| 77             | 1048           | 2011         | 2778         | 790 783              |
| 78             | 1049           |              |              |                      |
| 79             | 1050           | 2012         | 2779         | 790 27924            |
| 80             | 1051           | 2013         | 2780         | 789 5641             |
| 81             | 1052           | 2014         | 2781         | 791 4242             |
| 82             | 1053           |              |              |                      |
| 83             | 1054           | 2015         | 2782         | 789_6305             |
| 84             | 1055           | 2016         | 2783         | 790_1497             |
| 85             | 1056           |              |              |                      |
| 86             | 1057           | 2017         | 2784         | 788_13665            |
| 87             | 1058           | 2018         | 2785         | 790_9974             |
| 88             | 1059           | 2019         | 2786         | 784_1994             |
| 89             | 1060           | 2020         | 2787         | 784_3267             |
| 90             | 1061           | 2021         | 2788         | 784_13               |
| 91             | 1062           | 2022         | 2789         | 784_1536             |
| 92             | 1063           |              |              |                      |
| 93             | 1064           | 2023         | 2790         | 784_4084             |
| 94             | 1065           | 2024         | 2791         | 784_6206             |
| 95             | 1066           | 2025         | 2792         | 785_1300             |
| 96             | 1067           | 2026         | 2793         | 787_7605             |
| 97             | 1068           | 2027         | 2794         | 785_2429             |

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Table 6

| SEQ ID NO:     | SEQ ID NO:     | SEQ ID NO: | SEQ ID NO:   | Identification of                       |
|----------------|----------------|------------|--------------|-----------------------------------------|
| of full-length | of full-length | of contig  | of contig    | Priority Application                    |
| nucleotide     | peptide        | nucleotide | peptide      | that contig                             |
| sequence       | sequence       | sequence   | sequence     | nucleotide sequence                     |
|                |                |            |              | was filed (Attorney                     |
|                |                |            |              | Docket NoSEQ ID                         |
|                |                |            |              | NO.) *                                  |
| 98             | 1069           | 2028       | 2795         | 784_4076                                |
| 99             | 1070           | 2029       | 2796         | 784_10051                               |
| 100            | 1071           | 2030       | 2797         | 784_9491<br>784_4602                    |
| 101            | 1072           | 2031       | 2798<br>2799 | 784_4602                                |
| 102            | 1073           | 2032       | 2800         | 787 249                                 |
| 103            | 1074           | 2033       | 2800         | 767_249                                 |
| 104            | 1075           | 2024       | 2801         | 784 1700                                |
| 105            | 1076           | 2034       | 2802         | 787 2626                                |
| 106            | 1077           | 2035       |              | 792 1911                                |
| 107            | 1078           | 2036       | 2803<br>2804 | 784 8811                                |
| 108            | 1079           | 2038       | 2805         | 784 6218                                |
| 109            | 1080           | 2038       | 2806         | 789 5846                                |
| 110            |                | 2039       | 2807         | 784 3634                                |
| 111            | 1082<br>1083   | 2041       | 2808         | 787 5208                                |
|                |                | 2042       | 2809         | 787_3208                                |
| 113            | 1084           | 2042       |              | 788 8383                                |
| 114            | 1085           | 2044       | 2810<br>2811 | 784 8836                                |
| 115            | 1086           | 2045       | 2812         | 784 9029                                |
| 116            | 1087           | 2046       | 2813         | 784 8770                                |
| 117            | 1088           | 2046       | 2814         | 784 4083                                |
| 118            |                | 2047       | 2815         | 790 14642                               |
| 119            | 1090           | 2049       | 2816         | 784 4420                                |
| 121            | 1091           | 2050       | 2817         | 784 7113                                |
| 122            | 1092           | 2030       | 2017         | 704_7113                                |
| 123            | 1094           | 2051       | 2818         | 787 5474                                |
| 123            | 1095           | 2052       | 2819         | 784 1582                                |
| 125            | 1096           | 2032       | 2019         | 784_1382                                |
| 126            | 1097           | 2053       | 2820 .       | 784 8765                                |
| 127            | 1098           | 2054       | 2821         | 784_3761                                |
| 128            | 1098           | 2055       | 2822         | 784 8791                                |
| 129            | 1100           | 2056       | 2823         | 790 26782                               |
| 130            | 1100           | 2057       | 2824         | 785_2423                                |
| 131            | 1102           | 2058       | 2825         | 784 3090                                |
| 132            | 1102           | 2059       | 2826         | 784 5080                                |
| 133            | 1103           | 2007       | 2020         | 7.5.1_5000                              |
| 134            | 1105           | 2060       | 2827         | 787 3785                                |
| 135            | 1106           | 2061       | 2828         | 784 3091                                |
| 136            | 1107           | 2062       | 2829         | 784 3091                                |
| 137            | 1107           |            | 2022         | , 00071                                 |
| 138            | 1109           | 2063       | 2830         | 790 19641                               |
| 139            | 1110           | 2002       |              | ,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,, |
| 140            | 1111           | 2064       | 2831         | 790 2500                                |
| 141            | 1112           | 2065       | 2832         | 784 8758                                |
| 142            | 1113           | 2066       | 2833         | 784 1076                                |
| 143            | 1114           | 2067       | 2834         | 790 2608                                |
| 144            | 1115           | 2068       | 2835         | 784 4358                                |
| 145            | 1116           | 2069       | 2836         | 790_25033                               |
| 146            | 1117           | 2070       | 2837         | 784 2446                                |
| L140           | III/           | 20/0       | 1 2001       | 1 / 07 2770                             |

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Table 6

| SEQ ID NO:     | SEQ ID NO:     | SEQ ID NO:   | SEQ ID NO:   | Identification of           |
|----------------|----------------|--------------|--------------|-----------------------------|
| of full-length | of full-length | of contig    | of contig    | <b>Priority Application</b> |
| nucleotide     | peptide        | nucleotide   | peptide      | that contig                 |
| sequence       | sequence       | sequence     | sequence     | nucleotide sequence         |
|                |                |              |              | was filed (Attorney         |
|                |                |              |              | Docket NoSEQ ID             |
|                |                |              |              | NO.) *                      |
| 147            | 1118           | 2071         | 2838         | 784_1044                    |
| 148            | 1119           | 2072         | 2839         | 784_7636                    |
| 149            | 1120           | 2073         | 2840         | 787_134                     |
| 150            | 1121           | 2074         | 2841         | 791_2267                    |
| 151            | 1122           | 2075         | 2842         | 784_774                     |
| 152            | 1123           | 2076         | 2843         | 792_7564                    |
| 153            | 1124           | 2077         | 2844         | 784_9970                    |
| 154            | 1125           | 2050         |              |                             |
| 155            | 1126           | 2078         | 2845         | 784_3910                    |
| 156            | 1127           | 2070         | 2046         | 700 26052                   |
| 157            | 1128           | 2079         | 2846         | 790_26952                   |
| 158            | 1129           | 2080         | 2847         | 784_729                     |
| 159<br>160     | 1130           | 2081         | 2848         | 784_8218                    |
|                | 1131           | 2082         | 2849         | 784_8218                    |
| 161<br>162     | 1132<br>1133   | 2083         | 2850         | 784_4307                    |
| 163            | 1134           | 2004         | 2051         | 700 1062                    |
| 164            |                | 2084         | 2851         | 790_1063                    |
| 165            | 1135<br>1136   | 2085<br>2086 | 2852<br>2853 | 784_9448                    |
| 166            | 1137           |              | 2854         | 790_308<br>787_5972         |
| 167            | 1137           | 2087         | 2855         |                             |
| 168            | 1139           | 2000         | 2633         | 784_6680                    |
| 169            | 1140           |              |              |                             |
| 170            | 1141           | 2089         | 2856         | 784 4742                    |
| 171            | 1142           | 2090         | 2857         | 784 8152                    |
| 172            | 1143           | 2091         | 2858         | 789 5276                    |
| 173            | 1144           | 2092         | 2859         | 790 19423                   |
| 174            | 1145           | 2093         | 2860         | 784 3231                    |
| 175            | 1146           | 2093         | 2000         | 764_3231                    |
| 176            | 1147           | 2094         | 2861         | 790 19135                   |
| 177            | 1148           | 2095         | 2862         | 790_19133                   |
| 178            | 1149           | 2073         | 2002         | 190_2039                    |
| 179            | 1150           | 2096         | 2863         | 784_8713                    |
| 180            | 1151           | 2097         | 2864         | 790 15184                   |
| 181            | 1152           | 2098         | 2865         | 787 2134                    |
| 182            | 1153           | 2099         | 2866         | 784 4938                    |
| 183            | 1154           | 2000         | 2000         | 707_7730                    |
| 184            | 1155           | 2100         | 2867         | 784 1071                    |
| 185            | 1156           | 2101         | 2868         | 784 6181                    |
| 186            | 1157           | 2102         | 2869         | 784 193                     |
| 187            | 1157           | 2102         | 2870         | 790 24137                   |
| 188            | 1159           |              |              | 120_4T131                   |
| 189            | 1160           | 2104         | 2871         | 787 5326                    |
| 190            | 1161           | 2105         | 2872         | 784 1711                    |
| 191            | 1162           | 2106         | 2873         | 784 7239                    |
| 192            | 1163           | 2107         | 2874         | 784_3887                    |
| 193            | 1164           | 2108         | 2875         | 787 10175                   |
|                | 1165           | 2109         | 2876         | 792 6876                    |
| 194            | 1100           | 2102         |              | /9/ 08/0                    |

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Table 6

| SEQ ID NO:     | SEQ ID NO:     | SEQ ID NO:   | SEQ ID NO:   | Identification of         |
|----------------|----------------|--------------|--------------|---------------------------|
| of full-length | of full-length | of contig    | of contig    | Priority Application      |
| nucleotide     | peptide        | nucleotide   | peptide      | that contig               |
| sequence       | sequence       | sequence     | sequence     | nucleotide sequence       |
|                |                |              |              | was filed (Attorney       |
|                |                |              |              | Docket NoSEQ ID<br>NO.) * |
| 106            | 1167           | 0111         | 2070         | 788 12696                 |
| 196            | 1167           | 2111         | 2878<br>2879 | 784 183                   |
| 197            | 1168           | 2112         | 2880         | 784 9962                  |
| 198<br>199     | 1169<br>1170   | 2113         | 2881         | 790 11346                 |
| 200            | 1170           | 2114         | 2882         | 790_11346                 |
| 200            | 1172           | 2116         | 2883         | 784 3218                  |
| 202            | 1173           | 2117         | 2884         | 787 1179                  |
| 203            | 1174           | 2117         | 2885         | 784 8095                  |
| 204            | 1175           | 2119         | 2886         | 784 4778                  |
| 205            | 1176           | 2120         | 2887         | 784 815                   |
| 206            | 1177           | 2121         | 2888         | 792 633                   |
| 207            | 1178           | 2122         | 2889         | 784 5858                  |
| 208            | 1179           | 2123         | 2890         | 784 8485                  |
| 209            | 1180           | 2124         | 2891         | 784 5325                  |
| 210            | 1181           | 2125         | 2892         | 784 5417                  |
| 211            | 1182           | 2126         | 2893         | 788 13391                 |
| 212            | 1183           | 2127         | 2894         | 788 13391                 |
| 213            | 1184           | 2128         | 2895         | 784 2249                  |
| 214            | 1185           | 2129         | 2896         | 784 3755                  |
| 215            | 1186           | 2130         | 2897         | 785 540                   |
| 216            | 1187           | 2131         | 2898         | 787 5940                  |
| 217            | 1188           | 2132         | 2899         | 787 7631                  |
| 218            | 1189           | 2133         | 2900         | 791_4358                  |
| 219            | 1190           | 2134         | 2901         | 784_4277                  |
| 220            | 1191           | 2135         | 2902         | 787_10032                 |
| 221            | 1192           | 2136         | 2903         | 784_1775                  |
| 222            | 1193           |              |              |                           |
| 223            | 1194           | 2137         | 2904         | 784_2316                  |
| 224            | 1195           | 2138         | 2905         | 784_7495                  |
| 225            | 1196           | 2139         | 2906         | 784_7230                  |
| 226            | 1197           | 2140         | 2907         | 784_5855                  |
| 227            | 1198           | 2141         | 2908         | 785_828                   |
| 228            | 1199           | 2142         | 2909         | 787_4973                  |
| 229            | 1200           | 2143         | 2910         | 784_1993                  |
| 230            | 1201           | 2144         | 2911         | 790_3164                  |
| 231            | 1202           | 2145         | 2912         | 785_826                   |
| 232            | 1203           | <b> </b>     | 0010         | 704 4000                  |
| 233            | 1204           | 2146         | 2913         | 784_4003                  |
| 234            | 1205           | 2147         | 2914         | 788_12327                 |
| 235            | 1206           | 2148         | 2915         | 784_8963                  |
| 236            | 1207           | 2149         | 2916         | 785_3548                  |
| 237            | 1208           | 2150         | 2917         | 784_2151                  |
| 238            | 1209           | 2151         | 2918<br>2919 | 789_629<br>784_9496       |
| 239            | 1210           | 2152<br>2153 | 2919         | 784_9496<br>784_9496      |
| 240            | 1211           | 2153         | 2920         | 792 2014                  |
| 241            | 1212           | 2154         | 2721         | 174_4014                  |
| 242            | 1213           |              |              |                           |
| 243            | 1214           |              |              |                           |
| 244            | 1213           |              | 1            |                           |

1132

Table 6

| SEQ ID NO:     | SEQ ID NO:     | SEQ ID NO: | SEQ ID NO: | Identification of    |
|----------------|----------------|------------|------------|----------------------|
| of full-length | of full-length | of contig  | of contig  | Priority Application |
| nucleotide     | peptide        | nucleotide | peptide    | that contig          |
| sequence       | sequence       | sequence   | sequence   | nucleotide sequence  |
|                |                |            |            | was filed (Attorney  |
|                |                |            |            | Docket NoSEQ ID      |
|                |                |            |            | NO.) *               |
| 245            | 1216           | 2155       | 2922       | 784_5314             |
| 246            | 1217           | 2156       | 2923       | 792_4190             |
| 247            | 1218           | 2157       | 2924       | 787_8011             |
| 248            | 1219           | 2158       | 2925       | 784_8794             |
| 249            | 1220           | 2159       | 2926       | 784_2261             |
| 250            | 1221           | 2160       | 2927       | 788_4268             |
| 251            | 1222           | 2161       | 2928       | 784_9684             |
| 252            | 1223           | 2162       | 2929       | 784_2368             |
| 253            | 1224           | 2163       | 2930       | 784_7928             |
| 254            | 1225           | 2164       | 2931       | 784_1856             |
| 255            | 1226           | 2165       | 2932       | 784_6106             |
| 256            | 1227           | 2166       | 2933       | 784_6106             |
| 257            | 1228           | 2167       | 2934       | 784_1626             |
| 258            | 1229           | 2168       | 2935       | 784_4080             |
| 259            | 1230           | 2169       | 2936       | 784_194              |
| 260            | 1231           | 2170       | 2937       | 787_7988             |
| 261            | 1232           | 2171       | 2938       | 784_4707             |
| 262            | 1233           | 2172       | 2939       | 789_2100             |
| 263            | 1234           |            |            |                      |
| 264            | 1235           | 2173       | 2940       | 784_893              |
| 265            | 1236           | 2174       | 2941       | 789_1598             |
| 266            | 1237           | 2175       | 2942       | 784_834              |
| 267            | 1238           | 2176       | 2943       | 787_6026             |
| 268            | 1239           |            |            |                      |
| 269            | 1240           | 2177       | 2944       | 787_10200            |
| 270            | 1241           | 2178       | 2945       | 784_8799             |
| 271            | 1242           | 2179       | 2946       | 784_8340             |
| 272            | 1243           | 2180       | 2947       | 784_989              |
| 273            | 1244           | 2181       | 2948       | 788_5199             |
| 274            | 1245           |            |            |                      |
| 275            | 1246           | 2182       | 2949       | 787_6215             |
| 276            | 1247           | 2183       | 2950       | 784_2499             |
| 277            | 1248           | 2184       | 2951       | 784_3930             |
| 278            | 1249           | 2185       | 2952       | 784_3769             |
| 279            | 1250           | 2186       | 2953       | 784_2094             |
| 280            | 1251           | 2187       | 2954       | 785_1035             |
| 281            | 1252           |            |            |                      |
| 282            | 1253           | 2188       | 2955       | 784_9552             |
| 283            | 1254           | 2189       | 2956       | 784_9552             |
| 284            | 1255           | 2190       | 2957       | 790_21775            |
| 285            | 1256           | 2191       | 2958       | 785_3564             |
| 286            | 1257           | 2192       | 2959       | 784_1049             |
| 287            | 1258           | 2193       | 2960       | 790_19814            |
| 288            | 1259           | 2194       | 2961       | 784_1922             |
| 289            | 1260           | 2195       | 2962       | 784_4381             |
| 290            | 1261           | 2196       | 2963       | 784_1957             |
| 291            | 1262           | 2197       | 2964       | 787_5835             |
| 292            | 1263           | 2198       | 2965       | 787_5552             |
| 293            | 1264           | 2199       | 2966       | 784_9381             |

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Table 6

| SEQ ID NO:<br>of full-length<br>nucleotide<br>sequence | SEQ ID NO:<br>of full-length<br>peptide<br>sequence | SEQ ID NO:<br>of contig<br>nucleotide<br>sequence | SEQ ID NO:<br>of contig<br>peptide<br>sequence | Identification of Priority Application that contig nucleotide sequence was filed (Attorney Docket NoSEQ ID NO.) * |
|--------------------------------------------------------|-----------------------------------------------------|---------------------------------------------------|------------------------------------------------|-------------------------------------------------------------------------------------------------------------------|
| 294                                                    | 1265                                                |                                                   |                                                |                                                                                                                   |
| 295                                                    | 1266                                                | 2200                                              | 2967                                           | 788_10351                                                                                                         |
| 296                                                    | 1267                                                | 2201                                              | 2968                                           | 784_6729                                                                                                          |
| 297                                                    | 1268                                                | 2202                                              | 2969                                           | 784_2524                                                                                                          |
| 298                                                    | 1269                                                | 2203                                              | 2970                                           | 784_9087                                                                                                          |
| 299                                                    | 1270                                                | 2204                                              | 2971                                           | 788_13641                                                                                                         |
| 300                                                    | 1271                                                | 2205                                              | 2972                                           | 792_4273                                                                                                          |
| 301                                                    | 1272                                                | 2206                                              | 2973                                           | 784_8150                                                                                                          |
| 302                                                    | 1273                                                | 2207                                              | 2974                                           | 784_2159                                                                                                          |
| 303                                                    | 1274                                                | 2208                                              | 2975                                           | 784_9338                                                                                                          |
| 304                                                    | 1275                                                |                                                   |                                                |                                                                                                                   |
| 305                                                    | 1276                                                | 2209                                              | 2976                                           | 784_7665                                                                                                          |
| 306                                                    | 1277                                                | 2210                                              | 2977                                           | 784_2015                                                                                                          |
| 307                                                    | 1278                                                | 2211                                              | 2978                                           | 787_9885                                                                                                          |
| 308                                                    | 1279                                                | 2212                                              | 2979                                           | 790_14080                                                                                                         |
| 309                                                    | 1280                                                | 2213                                              | 2980                                           | 784_3052                                                                                                          |
| 310                                                    | 1281                                                |                                                   |                                                |                                                                                                                   |
| 311                                                    | 1282                                                | 2214                                              | 2981                                           | 784_1386                                                                                                          |
| 312                                                    | 1283                                                | 2215                                              | 2982                                           | 792_273                                                                                                           |
| 313                                                    | 1284                                                |                                                   |                                                |                                                                                                                   |
| 314                                                    | 1285                                                |                                                   |                                                |                                                                                                                   |
| 315                                                    | 1286                                                | 2216                                              | 2983                                           | 792_6952                                                                                                          |
| 316                                                    | 1287                                                | 2217                                              | 2984                                           | 784_3783                                                                                                          |
| 317                                                    | 1288                                                | 2218                                              | 2985                                           | 784_3783                                                                                                          |
| 318                                                    | 1289                                                |                                                   |                                                |                                                                                                                   |
| 319                                                    | 1290                                                | 2219                                              | 2986                                           | 790_1199                                                                                                          |
| 320                                                    | 1291                                                | 2220                                              | 2987                                           | 792_5495                                                                                                          |
| 321                                                    | 1292                                                | 2221                                              | 2988                                           | 784_2270                                                                                                          |
| 322                                                    | 1293                                                | 2222                                              | 2989                                           | 784_1824                                                                                                          |
| 323                                                    | 1294                                                | 2223                                              | 2990                                           | 787_5550                                                                                                          |
| 324                                                    | 1295                                                | 2224                                              | 2991                                           | 790_27374                                                                                                         |
| 325                                                    | 1296                                                |                                                   |                                                |                                                                                                                   |
| 326                                                    | 1297                                                | 2225                                              | 2992                                           | 790_14323                                                                                                         |
| 327                                                    | 1298                                                |                                                   |                                                |                                                                                                                   |
| 328                                                    | 1299                                                |                                                   |                                                |                                                                                                                   |
| 329                                                    | 1300                                                | 2226                                              | 2993                                           | 784_8128                                                                                                          |
| 330                                                    | 1301                                                | 2227                                              | 2994                                           | 784_9591                                                                                                          |
| 331                                                    | 1302                                                | 2228                                              | 2995                                           | 784_7674                                                                                                          |
| 332                                                    | 1303                                                | 2229                                              | 2996                                           | 784_3111                                                                                                          |
| 333                                                    | 1304                                                | 2230                                              | 2997                                           | 790_22977                                                                                                         |
| 334                                                    | 1305 .                                              | 2231                                              | 2998                                           | 784_1073                                                                                                          |
| 335                                                    | 1306                                                | 2232                                              | 2999                                           | 784_636                                                                                                           |
| 336                                                    | 1307                                                | 2233                                              | 3000                                           | 784_6892                                                                                                          |
| 337                                                    | 1308                                                | 2234                                              | 3001                                           | 789_658                                                                                                           |
| 338                                                    | 1309                                                | 2235                                              | 3002                                           | 790_2458                                                                                                          |
| 339                                                    | 1310                                                | 2236                                              | 3003                                           | 792_4252                                                                                                          |
| 340                                                    | 1311                                                | 2237                                              | 3004                                           | 787_10241                                                                                                         |
| 341                                                    | 1312                                                | 2238                                              | 3005                                           | 784_4656                                                                                                          |
| 342                                                    | 1313                                                | 2239                                              | 3006                                           | 784_7738                                                                                                          |

1134 .

Table 6

| SEQ ID NO:     | SEQ ID NO:     | SEQ ID NO: | SEQ ID NO: | Identification of    |
|----------------|----------------|------------|------------|----------------------|
| of full-length | of full-length | of contig  | of contig  | Priority Application |
| nucleotide     | peptide        | nucleotide | peptide    | that contig          |
| sequence       | sequence       | sequence   | sequence   | nucleotide sequence  |
| _              | _              | _          | _          | was filed (Attorney  |
|                |                |            |            | Docket NoSEQ ID      |
|                |                |            |            | NO.) *               |
| 343            | 1314           |            |            |                      |
| 344            | 1315           | 2240       | 3007       | 784_3494             |
| 345            | 1316           | 2241       | 3008       | 784_7572             |
| 346            | 1317           | 2242       | 3009       | 784_2401             |
| 347            | 1318           | 2243       | 3010       | 787_2452             |
| 348            | 1319           | 2244       | 3011       | 784_9487             |
| 349            | 1320           | 2245       | 3012       | 784_2664             |
| 350            | 1321           |            |            |                      |
| 351            | 1322           | 2246       | 3013       | 787_7317             |
| 352            | 1323           | 2247       | 3014       | 790_10590            |
| 353            | 1324           | 2248       | 3015       | 789_4906             |
| 354            | 1325           |            |            |                      |
| 355            | 1326           | 2249       | 3016       | 784_10280            |
| 356            | 1327           | 2250       | 3017       | 787_2292             |
| 357            | 1328           | 2251       | 3018       | 785_364              |
| 358            | 1329           | 2252       | 3019       | 784_4447             |
| 359            | 1330           | 2253       | 3020       | 787_8910             |
| 360            | 1331           | 2254       | 3021       | 784_9704             |
| 361            | 1332           |            |            |                      |
| 362            | 1333           | 2255       | 3022       | 784_2063             |
| 363            | 1334           | 2256       | 3023       | 784_1972             |
| 364            | 1335           | 2257       | 3024       | 784_6431             |
| 365            | 1336           | 2258       | 3025       | 784_6001             |
| 366            | 1337           | 2259       | 3026       | 784_6950             |
| 367            | 1338           | 2260       | 3027       | 790_5583             |
| 368            | 1339           | 2261       | 3028       | 784_1305             |
| 369            | 1340           | 2262       | 3029       | 790_5747             |
| 370            | 1341           | 2263       | 3030       | 784_6493             |
| 371            | 1342           |            |            |                      |
| 372            | 1343           | 2264       | 3031       | 790_14586            |
| 373            | 1344           | 2265       | 3032       | 787_2133             |
| 374            | 1345           | 2266       | 2000       | 500 1010             |
| 375            | 1346           | 2266       | 3033       | 788_4349             |
| 376            | 1347           | 2267       | 3034       | 787_10237            |
| 377            | 1348           | 2262       | 2025       | 504.054              |
| 378            | 1349           | 2268       | 3035       | 784_254              |
| 379            | 1350           | 2262       | 2026       | mo.4. 5001           |
| 380            | 1351           | 2269       | 3036       | 784_5321             |
| 381            | 1352           | 2270       | 3037       | 791_1515             |
| 382            | 1353           | 2271       | 3038       | 787_9061             |
| 383            | 1354           | 2272       | 3039       | 784_7513             |
| 384            | 1355           | 2273       | 3040       | 787_3196             |
| 385            | 1356           | 2274       | 3041       | 788_13324            |
| 386            | 1357           |            |            |                      |
| 387            | 1358           | 2075       | 2042       | 504 0074             |
| 388            | 1359           | 2275       | 3042       | 784_2074             |
| 389            | 1360           | 2276       | 3043       | 787_5928             |
| 390            | 1361           | 2277       | 3044       | 784_2322             |
| 391            | 1362           | 2278       | 3045       | 790_12083            |

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Table 6

| SEQ ID NO:<br>of full-length<br>nucleotide<br>sequence | SEQ ID NO:<br>of full-length<br>peptide<br>sequence | SEQ ID NO:<br>of contig<br>nucleotide<br>sequence | SEQ ID NO:<br>of contig<br>peptide<br>sequence | Identification of Priority Application that contig nucleotide sequence was filed (Attorney Docket NoSEQ ID NO.) * |
|--------------------------------------------------------|-----------------------------------------------------|---------------------------------------------------|------------------------------------------------|-------------------------------------------------------------------------------------------------------------------|
| 392                                                    | 1363                                                | 2279                                              | 3046                                           | 784_4511                                                                                                          |
| 393                                                    | 1364                                                | 2280                                              | 3047                                           | 790_1886                                                                                                          |
| 394                                                    | 1365                                                |                                                   |                                                |                                                                                                                   |
| 395                                                    | 1366                                                | 2281                                              | 3048                                           | 784_232                                                                                                           |
| 396                                                    | 1367                                                | 2282                                              | 3049                                           | 784_1884                                                                                                          |
| 397                                                    | 1368                                                |                                                   |                                                |                                                                                                                   |
| 398                                                    | 1369                                                | 2283                                              | 3050                                           | 784_2082                                                                                                          |
| 399                                                    | 1370                                                | 2284                                              | 3051                                           | 790_24248                                                                                                         |
| 400                                                    | 1371                                                | 2285                                              | 3052                                           | 784_3847                                                                                                          |
| 401                                                    | 1372                                                | 2286                                              | 3053                                           | 790_21352                                                                                                         |
| 402                                                    | 1373                                                |                                                   |                                                |                                                                                                                   |
| 403                                                    | 1374                                                | 2287                                              | 3054                                           | 787_7127                                                                                                          |
| 404                                                    | 1375                                                | 2288                                              | 3055                                           | 784_5344                                                                                                          |
| 405                                                    | 1376                                                | 2289                                              | 3056                                           | 787_10040                                                                                                         |
| 406                                                    | 1377                                                | 2290                                              | 3057                                           | 790_15388                                                                                                         |
| 407                                                    | 1378                                                | 2291                                              | 3058                                           | 784_2116                                                                                                          |
| 408                                                    | 1379                                                | 2292                                              | 3059                                           | 784_10202                                                                                                         |
| 409                                                    | 1380                                                |                                                   |                                                |                                                                                                                   |
| 410                                                    | 1381                                                | 2293                                              | 3060                                           | 784_5329                                                                                                          |
| 411                                                    | 1382                                                | 2294                                              | 3061                                           | 784_5329                                                                                                          |
| 412                                                    | 1383                                                | 2295                                              | 3062                                           | 784_5329                                                                                                          |
| 413                                                    | 1384                                                | 2296                                              | 3063                                           | 784_1921                                                                                                          |
| 414                                                    | 1385                                                | 2297                                              | 3064                                           | 784_8888                                                                                                          |
| 415                                                    | 1386                                                | 2298                                              | 3065                                           | 784_6518                                                                                                          |
| 416                                                    | 1387                                                | 2299                                              | 3066                                           | 788_5134                                                                                                          |
| 417                                                    | 1388                                                |                                                   |                                                |                                                                                                                   |
| 418                                                    | 1389                                                | 2300                                              | 3067                                           | 789_439                                                                                                           |
| 419                                                    | 1390                                                |                                                   |                                                |                                                                                                                   |
| 420                                                    | 1391                                                | 2301                                              | 3068                                           | 784_2147                                                                                                          |
| 421                                                    | 1392                                                | 2302                                              | 3069                                           | 787_8778                                                                                                          |
| 422                                                    | 1393                                                | 2303                                              | 3070                                           | 790_2428                                                                                                          |
| 423                                                    | 1394                                                |                                                   |                                                |                                                                                                                   |
| 424                                                    | 1395                                                | 2304                                              | 3071                                           | 787_1365                                                                                                          |
| 425                                                    | 1396                                                | 2305                                              | 3072                                           | 790_15951                                                                                                         |
| 426                                                    | 1397                                                | 2306                                              | 3073                                           | 784_9724                                                                                                          |
| 427                                                    | 1398                                                |                                                   |                                                |                                                                                                                   |
| 428                                                    | 1399                                                |                                                   |                                                |                                                                                                                   |
| 429                                                    | 1400                                                |                                                   |                                                |                                                                                                                   |
| 430                                                    | 1401                                                | 2307                                              | 3074                                           | 790_16631                                                                                                         |
| 431                                                    | 1402                                                | 2308                                              | 3075                                           | 790_1660                                                                                                          |
| 432                                                    | 1403                                                | 2309                                              | 3076                                           | 787_1694                                                                                                          |
| 433                                                    | 1404                                                | 2310                                              | 3077                                           | 790_9736                                                                                                          |
| 434                                                    | 1405                                                | 2311                                              | 3078                                           | 790_19371                                                                                                         |
| 435                                                    | 1406                                                |                                                   |                                                |                                                                                                                   |
| 436                                                    | 1407                                                |                                                   |                                                |                                                                                                                   |
| 437                                                    | 1408                                                | 2312                                              | 3079                                           | 784_5732                                                                                                          |
| 438                                                    | 1409                                                | 2313                                              | 3080                                           | 790_28173                                                                                                         |
| 439                                                    | 1410                                                | 2314                                              | 3081                                           | 787_8248                                                                                                          |
| 440                                                    | 1411                                                | 2315                                              | 3082                                           | 787_7219                                                                                                          |

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Table 6

| SEQ ID NO:<br>of full-length<br>nucleotide<br>sequence | SEQ ID NO:<br>of full-length<br>peptide<br>sequence | SEQ ID NO: of contig nucleotide sequence | SEQ ID NO:<br>of contig<br>peptide<br>sequence | Identification of Priority Application that contig nucleotide sequence was filed (Attorney Docket NoSEQ ID NO.) * |
|--------------------------------------------------------|-----------------------------------------------------|------------------------------------------|------------------------------------------------|-------------------------------------------------------------------------------------------------------------------|
| 441                                                    | 1412                                                | 2316                                     | 3083                                           | 791 634                                                                                                           |
| 442                                                    | 1413                                                | 2317                                     | 3084                                           | 791 401                                                                                                           |
| 443                                                    | 1414                                                | 2318                                     | 3085                                           | 784 5558                                                                                                          |
| 444                                                    | 1415                                                | 2319                                     | 3086                                           | 784 2037                                                                                                          |
| 445                                                    | 1416                                                |                                          |                                                |                                                                                                                   |
| 446                                                    | 1417                                                | 2320                                     | 3087                                           | 784 10005                                                                                                         |
| 447                                                    | 1418                                                | 2321                                     | 3088                                           | 784 10064                                                                                                         |
| 448                                                    | 1419                                                | 2322                                     | 3089                                           | 784 10064                                                                                                         |
| 449                                                    | 1420                                                | 2323                                     | 3090                                           | 787 10073                                                                                                         |
| 450                                                    | 1421                                                | 2324                                     | 3091                                           | 789 644                                                                                                           |
| 451                                                    | 1422                                                | 2325                                     | 3092                                           | 784 2292                                                                                                          |
| 452                                                    | 1423                                                |                                          |                                                |                                                                                                                   |
| 453                                                    | 1424                                                | 2326                                     | 3093                                           | 784 9391                                                                                                          |
| 454                                                    | 1425                                                | 2327                                     | 3094                                           | 787 9807                                                                                                          |
| 455                                                    | 1426                                                | 2328                                     | 3095                                           | 784 8920                                                                                                          |
| 456                                                    | 1427                                                |                                          |                                                |                                                                                                                   |
| 457                                                    | 1428                                                | 2329                                     | 3096                                           | 784 4699                                                                                                          |
| 458                                                    | 1429                                                |                                          |                                                |                                                                                                                   |
| 459                                                    | 1430                                                | 2330                                     | 3097                                           | 784 908                                                                                                           |
| 460                                                    | 1431                                                | 2331                                     | 3098                                           | 787 5515                                                                                                          |
| 461                                                    | 1432                                                | 2332                                     | 3099                                           | 787 7919                                                                                                          |
| 462                                                    | 1433                                                | 2333                                     | 3100                                           | 789 2723                                                                                                          |
| 463                                                    | 1434                                                | 2334                                     | 3101                                           | 784 1807                                                                                                          |
| 464                                                    | 1435                                                | 2335                                     | 3102                                           | 790 8144                                                                                                          |
| 465                                                    | 1436                                                | 2336                                     | 3103                                           | 784 9640                                                                                                          |
| 466                                                    | 1437                                                | 2337                                     | 3104                                           | 787 5310                                                                                                          |
| 467                                                    | 1438                                                | 2338                                     | 3105                                           | 790 11190                                                                                                         |
| 468                                                    | 1439                                                | 2339                                     | 3106                                           | 787 9200                                                                                                          |
| 469                                                    | 1440                                                | 2340                                     | 3107                                           | 790 15075                                                                                                         |
| 470                                                    | 1441                                                | 2341                                     | 3108                                           | 784 531                                                                                                           |
| 471                                                    | 1442                                                | 2342                                     | 3109                                           | 792_7587                                                                                                          |
| 472                                                    | 1443                                                | 2343                                     | 3110                                           | 784_10061                                                                                                         |
| 473                                                    | 1444                                                | 2344                                     | 3111                                           | 790_3597                                                                                                          |
| 474                                                    | 1445                                                |                                          |                                                |                                                                                                                   |
| 475                                                    | 1446                                                | 2345                                     | 3112                                           | 787_161                                                                                                           |
| 476                                                    | 1447                                                |                                          |                                                |                                                                                                                   |
| 477                                                    | 1448                                                |                                          |                                                |                                                                                                                   |
| 478                                                    | 1449                                                | 2346                                     | 3113                                           | 790_11842                                                                                                         |
| 479                                                    | 1450                                                | 2347                                     | 3114                                           | 784_5654                                                                                                          |
| 480                                                    | 1451                                                | 2348                                     | 3115                                           | 787_3486                                                                                                          |
| 481                                                    | 1452                                                | 2349                                     | 3116                                           | 792_7587                                                                                                          |
| 482                                                    | 1453                                                | 2350                                     | 3117                                           | 784_8992                                                                                                          |
| 483                                                    | 1454                                                | 2351                                     | 3118                                           | 784_4957                                                                                                          |
| 484                                                    | 1455                                                |                                          |                                                |                                                                                                                   |
| 485                                                    | 1456                                                | 2352                                     | 3119                                           | 790_1917                                                                                                          |
| 486                                                    | 1457                                                |                                          |                                                |                                                                                                                   |
| 487                                                    | 1458                                                |                                          |                                                |                                                                                                                   |
| 488                                                    | 1459                                                | 2353                                     | 3120                                           | 787_3947                                                                                                          |
| 489                                                    | 1460                                                | 2354                                     | 3121                                           | 784_6581                                                                                                          |

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Table 6

| SEQ ID NO:     | SEQ ID NO:     | SEQ ID NO: | SEQ ID NO: | Identification of      |
|----------------|----------------|------------|------------|------------------------|
| of full-length | of full-length | of contig  | of contig  | Priority Application   |
| nucleotide     | peptide        | nucleotide | peptide    | that contig            |
| sequence       | sequence       | sequence   | sequence   | nucleotide sequence    |
|                |                |            |            | was filed (Attorney    |
|                |                |            |            | Docket NoSEQ ID NO.) * |
| 490            | 1461           |            |            | NO.) "                 |
| 491            | 1462           | 2355       | 3122       | 784 1691               |
| 492            | 1463           | 2333       | 3122       | 70107                  |
| 493            | 1464           | 2356       | 3123       | 790 15794              |
| 494            | 1465           | 2357       | 3124       | 784 3609               |
| 495            | 1466           | 2358       | 3125       | 787 4906               |
| 496            | 1467           | 2359       | 3126       | 790 1952               |
| 497            | 1468           | 2360       | 3127       | 790 3855               |
| 498            | 1469           | 2361       | 3128       | 787 4361               |
| 499            | 1470           | 2362       | 3129       | 787 2551               |
| 500            | 1471           | 2302       |            |                        |
| 501            | 1472           | 2363       | 3130       | 788_3778               |
| 502            | 1473           | 2364       | 3131       | 790 29526              |
| 503            | 1474           | 2365       | 3132       | 784 10066              |
| 504            | 1475           | 2366       | 3133       | 784 10066              |
| 505            | 1476           | 2367       | 3134       | 787 9841               |
| 506            | 1477           | 2368       | 3135       | 787 2410               |
| 507            | 1478           | 2369       | 3136       | 790 12704              |
| 508            | 1479           | 230)       | 3130       |                        |
| 509            | 1480           | 2370       | 3137       | 790 6209               |
| 510            | 1481           | 2371       | 3138       | 789 3411               |
| 511            | 1482           | 2372       | 3139       | 784 9888               |
| 512            | 1483           | 2373       | 3140       | 790 29516              |
| 513            | 1484           | 2010       |            |                        |
| 514            | 1485           | 2374       | 3141       | 784 6670               |
| 515            | 1486           | 2375       | 3142       | 785 555                |
| 516            | 1487           | 2376       | 3143       | 790 10968              |
| 517            | 1488           | 2377       | 3144       | 787 5633               |
| 518            | 1489           | 2378       | 3145       | 784 9133               |
| 519            | 1490           | 2379       | 3146       | 784 6391               |
| 520            | 1491           |            |            |                        |
| 521            | 1492           | 2380       | 3147       | 787 6115               |
| 522            | 1493           | 2381       | 3148       | 784 2126               |
| 523            | 1494           | 2382       | 3149       | 784 8754               |
| 524            | 1495           | 2383       | 3150       | 790_14360              |
| 525            | 1496           | 2384       | 3151       | 787_9248               |
| 526            | 1497           | 2385       | 3152       | 787_4445               |
| 527            | 1498           | 2386       | 3153       | 787_5648               |
| 528            | 1499           | 2387       | 3154       | 790_22816              |
| 529            | 1500           |            | T          |                        |
| 530            | 1501           |            |            |                        |
| 531            | 1502           | 2388       | 3155       | 788 9557               |
| 532            | 1503           | 2389       | 3156       | 784 7364               |
| 533            | 1504           | 2390       | 3157       | 787 10184              |
| 534            | 1505           | 2391       | 3158       | 790 1148               |
| 535            | 1506           |            |            |                        |
| 536            | 1507           | 2392       | 3159       | 788 5424               |
| 537            | 1508           | 2393       | 3160       | 787_10099              |
| 538            | 1509           |            |            |                        |

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Table 6

| SEQ ID NO:     | SEQ ID NO:     | SEQ ID NO: | SEQ ID NO:          | Identification of               |
|----------------|----------------|------------|---------------------|---------------------------------|
| of full-length | of full-length | of contig  | of contig           | Priority Application            |
| nucleotide     | peptide        | nucleotide | peptide<br>sequence | that contig nucleotide sequence |
| sequence       | sequence       | sequence   | sequence            | was filed (Attorney             |
|                |                |            |                     | Docket No. SEQ ID               |
|                |                |            |                     | NO.) *                          |
| 539            | 1510           |            |                     | 1,0,0                           |
| 540            | 1511           |            |                     | ***                             |
| 541            | 1512           | 2394       | 3161                | 784_10185                       |
| 542            | 1513           | 2395       | 3162                | 784_3322                        |
| 543            | 1514           | 2396       | 3163                | 784_1553                        |
| 544            | 1515           | 2397       | 3164                | 790_19723                       |
| 545            | 1516           |            |                     |                                 |
| 546            | 1517           | 2398       | 3165                | 787_813                         |
| 547            | 1518           | 2399       | 3166                | 790_16130                       |
| 548            | 1519           | 2400       | 3167                | 784_972                         |
| 549            | 1520           | 2401       | 3168                | 790_23073                       |
| 550            | 1521           | 2402       | 3169                | 784_5293                        |
| 551            | 1522           | 2403       | 3170                | 784_3041                        |
| 552            | 1523           | 2404       | 3171                | 784_5365                        |
| 553            | 1524           | 2405       | 3172                | 790_11131                       |
| 554            | 1525           | 2406       | 3173                | 787_3748                        |
| 555            | 1526           | 2407       | 3174                | 789_4975                        |
| 556            | 1527           | 2408       | 3175                | 787_3743                        |
| 557            | 1528           | 2409       | 3176                | 787_3743                        |
| 558            | 1529           |            |                     |                                 |
| 559            | 1530           | 2410       | 3177                | 787_2855                        |
| 560            | 1531           | 2411       | 3178                | 787_2447                        |
| 561            | 1532           | 2412       | 3179                | 784_9156                        |
| 562            | 1533           |            |                     |                                 |
| 563            | 1534           | 2413       | 3180                | 784_7447                        |
| 564            | 1535           | 2414       | 3181                | 784_7447                        |
| 565            | 1536           | 2415       | 3182                | 790_18202                       |
| 566            | 1537           | 2416       | 3183                | 789_1599                        |
| 567            | 1538           | 2417       | 3184                | 784_4033                        |
| 568            | 1539           | 2418       | 3185                | 784_5329                        |
| 569            | 1540           | 2419       | 3186                | 790_10614                       |
| 570            | 1541           | 2420       | 3187                | 784_5434                        |
| 571            | 1542           | 2421       | 3188                | 784_9815                        |
| 572            | 1543           | 2422       | 3189                | 787_2513                        |
| 573            | 1544           |            |                     |                                 |
| 574            | 1545           | 0.422      | 2100                | 704 5029                        |
| 575            | 1546           | 2423       | 3190                | 784_5038                        |
| 576            | 1547           | 2424       | 3191                | 784_1339                        |
| 577            | 1548           | 2425       | 3192                | 784_3599                        |
| 578            | 1549           | 2426       | 2102                | 790 12410                       |
| 579            | 1550           | 2426       | 3193                | /30_12410                       |
| 580            | 1551           |            | <del> </del>        |                                 |
| 581            | 1552           |            |                     |                                 |
| 582            | 1553<br>1554   | 2427       | 2104                | 784 1927                        |
| 583            | 1555           | 2427       | 3194                | 790 26548                       |
| 584            | 1556           | 2428       | 3195                | 790_20348                       |
| 585            | 1557           | 2429       | 3196                | 790 7287                        |
| 586            |                |            | 3197                | 790_7287                        |
| 587            | 1558           | 2431       | 3198                | /90_13000                       |

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Table 6

| SEQ ID NO:     | SEQ ID NO:     | SEQ ID NO: | SEQ ID NO: | Identification of                       |
|----------------|----------------|------------|------------|-----------------------------------------|
| of full-length | of full-length | of contig  | of contig  | Priority Application                    |
| nucleotide     | peptide        | nucleotide | peptide    | that contig                             |
| sequence       | sequence       | sequence   | sequence   | nucleotide sequence                     |
|                |                |            |            | was filed (Attorney                     |
|                |                |            |            | Docket NoSEQ ID                         |
| 500            | 1559           | 2432       | 3199       | NO.) *                                  |
| 588<br>589     | 1560           | 2432       | 3200       | 790 6409                                |
| 590            | 1561           | 2434       | 3200       | 787 2322                                |
| 591            | 1562           | 2434       | 3201       | 101_2322                                |
| 592            | 1563           | 2435       | 3202       | 784 8245                                |
| 593            | 1564           | 2436       | 3203       | 784 8245                                |
| 594            | 1565           | 2437       | 3204       | 790 15575                               |
| 595            | 1566           | 2137       | 1 3201     | ,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,, |
| 596            | 1567           |            |            |                                         |
| 597            | 1568           |            |            |                                         |
| 598            | 1569           | 2438       | 3205       | 784 7955                                |
| 599            | 1570           | 2439       | 3206       | 787 2691                                |
| 600            | 1571           | 2440       | 3207       | 787 5853                                |
| 601            | 1572           | 2441       | 3208       | 787 10136                               |
| 602            | 1573           | 2442       | 3209       | 784 8360                                |
| 603            | 1574           | 2443       | 3210       | 790 22260                               |
| 604            | 1575           |            | 1          |                                         |
| 605            | 1576           | 2444       | 3211       | 784_2677                                |
| 606            | 1577           | 2445       | 3212       | 784 8042                                |
| 607            | 1578           | 2446       | 3213       | 789 6361                                |
| 608            | 1579           | 2447       | 3214       | 784 5150                                |
| 609            | 1580           |            |            |                                         |
| 610            | 1581           |            |            |                                         |
| 611            | 1582           | 2448       | 3215       | 784 3279                                |
| 612            | 1583           |            |            |                                         |
| 613            | 1584           | 2449       | 3216       | 790 28630                               |
| 614            | 1585           | 2450       | 3217       | 784_1238                                |
| 615            | 1586           | 2451       | 3218       | 787_9483                                |
| 616            | 1587           | 2452       | 3219       | 787_4499                                |
| 617            | 1588           |            |            |                                         |
| 618            | 1589           |            |            |                                         |
| 619            | 1590           | 2453       | 3220       | 790_2304                                |
| 620            | 1591           | 2454       | 3221       | 791_1303                                |
| 621            | 1592           | 2455       | 3222       | 791_1303                                |
| 622            | 1593           |            |            |                                         |
| 623            | 1594           | 2456       | 3223       | 790_16004                               |
| 624            | 1595           |            |            |                                         |
| 625            | 1596           | 2457       | 3224       | 790_11182                               |
| 626            | 1597           | 2458       | 3225       | 784_1981                                |
| 627            | 1598           |            |            |                                         |
| 628            | 1599           |            |            |                                         |
| 629            | 1600           | 2459       | 3226       | 784_1026                                |
| 630            | 1601           |            |            |                                         |
| 631            | 1602           | 2460       | 3227       | 790_16240                               |
| 632            | 1603           | 2461       | 3228       | 790_14734                               |
| 633            | 1604           |            |            |                                         |
| 634            | 1605           |            |            |                                         |
| 635            | 1606           | 2462       | 3229       | 784_9753                                |
| 636            | 1607           | 2463       | 3230       | 789_5821                                |

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Table 6

| SEQ ID NO:                            | SEQ ID NO:     | SEQ ID NO:   | SEQ ID NO:   | Identification of                     |
|---------------------------------------|----------------|--------------|--------------|---------------------------------------|
| of full-length                        | of full-length | of contig    | of contig    | Priority Application                  |
| nucleotide                            | peptide        | nucleotide   | peptide      | that contig                           |
| sequence                              | sequence       | sequence     | sequence     | nucleotide sequence                   |
|                                       |                |              |              | was filed (Attorney Docket No. SEQ ID |
|                                       |                |              |              | NO.) *                                |
| 637                                   | 1608           |              |              | 110.)                                 |
| 638                                   | 1609           |              |              |                                       |
| 639                                   | 1610           | 2464         | 3231         | 788 2614                              |
| 640                                   | 1611           |              |              |                                       |
| 641                                   | 1612           | 2465         | 3232         | 784 4769                              |
| 642                                   | 1613           | 2466         | 3233         | 784_4769                              |
| 643                                   | 1614           | 2467         | 3234         | 784_2968                              |
| 644                                   | 1615           | 2468         | 3235         | 784_142                               |
| 645                                   | 1616           | 2469         | 3236         | 784_5903                              |
| 646                                   | 1617           | 2470         | 3237         | 784_7930                              |
| 647                                   | 1618           |              |              |                                       |
| 648                                   | 1619           | 2471         | 3238         | 784_3247                              |
| 649                                   | 1620           | 2472         | 3239         | 784_3247                              |
| 650                                   | 1621           | 2473         | 3240         | 787_2820                              |
| 651                                   | 1622           | 2474         | 3241         | 784_10030                             |
| 652                                   | 1623           | 2475         | 3242         | 784_10050                             |
| 653                                   | 1624           | 2476         | 3243         | 784_1136                              |
| 654                                   | 1625           | 2477         | 3244         | 790_3151                              |
| 655                                   | 1626           | 2478         | 3245         | 784_4242                              |
| 656                                   | 1627           | 2479         | 3246         | 791_4309                              |
| 657                                   | 1628           | 2480         | 3247         | 790_3196                              |
| 658                                   | 1629           | 2481         | 3248         | 790_28262                             |
| 659                                   | 1630           | 2482         | 3249         | 784_3774                              |
| 660                                   | 1631           | 2483         | 3250         | 784_1361                              |
| 661                                   | 1632           |              |              | 504 5610                              |
| 662                                   | 1633           | 2484         | 3251         | 784_5612                              |
| 663                                   | 1634           | 2485         | 3252         | 784_3593                              |
| 664                                   | 1635           | 0.10.6       | 2252         | 700 1613                              |
| 665                                   | 1636           | 2486         | 3253         | 789_1613                              |
| 666                                   | 1637           |              |              |                                       |
| 667                                   | 1638           | 2407         | 2254         | 790 25912                             |
| 668<br>669                            | 1639<br>1640   | 2487<br>2488 | 3254<br>3255 | 787 10217                             |
|                                       |                |              |              | 784 6584                              |
| 670<br>671                            | 1641<br>1642   | 2489<br>2490 | 3256<br>3257 | 784 5348                              |
| 672                                   | 1643           | 2491         | 3257         | 785 1029                              |
| 673                                   | 1644           | 2491         | 3259         | 784 1517                              |
| 674                                   | 1645           | L772         | 3439         | ,07_131/                              |
| 675                                   | 1646           | 2493         | 3260         | 787 766                               |
| 676                                   | 1647           | 2494         | 3261         | 784 10155                             |
| 677                                   | 1648           | 2495         | 3262         | 790 26542                             |
| 678                                   | 1649           | 2496         | 3263         | 787 5996                              |
| 679                                   | 1650           | 1            | 2203         |                                       |
| 680                                   | 1651           | 2497         | 3264         | 785 3492                              |
| 681                                   | 1652           | 2498         | 3265         | 784 5074                              |
| 682                                   | 1653           | 2499         | 3266         | 787 10214                             |
| · · · · · · · · · · · · · · · · · · · | 1 1033         |              |              |                                       |
| 683                                   |                |              | 3267         | 784 5399                              |
| 683<br>684                            | 1654<br>1655   | 2500         | 3267         | 784_5399                              |

1141

Table 6

| SEQ ID NO:<br>of full-length<br>nucleotide<br>sequence | SEQ ID NO:<br>of full-length<br>peptide<br>sequence | SEQ ID NO:<br>of contig<br>nucleotide<br>sequence | SEQ ID NO:<br>of contig<br>peptide<br>sequence | Identification of Priority Application that contig nucleotide sequence was filed (Attorney |
|--------------------------------------------------------|-----------------------------------------------------|---------------------------------------------------|------------------------------------------------|--------------------------------------------------------------------------------------------|
|                                                        |                                                     |                                                   |                                                | Docket NoSEQ ID<br>NO.) *                                                                  |
| 686                                                    | 1657                                                |                                                   |                                                |                                                                                            |
| 687                                                    | 1658                                                | 2502                                              | 3269                                           | 790_15978                                                                                  |
| 688                                                    | 1659                                                | 2503                                              | 3270                                           | 790_11139                                                                                  |
| 689                                                    | 1660                                                | 2504                                              | 3271                                           | 784_2833                                                                                   |
| 690                                                    | 1661                                                | 2505                                              | 3272                                           | 787_4050                                                                                   |
| 691                                                    | 1662                                                | 2506                                              | 3273                                           | 787_6078                                                                                   |
| 692                                                    | 1663                                                |                                                   |                                                |                                                                                            |
| 693                                                    | 1664                                                | 2507                                              | 3274                                           | 790_3691                                                                                   |
| 694                                                    | 1665                                                |                                                   | 225                                            | 504 0205                                                                                   |
| 695                                                    | 1666                                                | 2508                                              | 3275                                           | 784_2305                                                                                   |
| 696                                                    | 1667                                                | 2509                                              | 3276                                           | 784_2305                                                                                   |
| 697                                                    | 1668                                                | 2510                                              | 3277                                           | 790_195                                                                                    |
| 698                                                    | 1669                                                | 2511                                              | 3278                                           | 784_3569                                                                                   |
| 699                                                    | 1670                                                |                                                   |                                                |                                                                                            |
| 700                                                    | 1671                                                | 2512                                              | 3279                                           | 785 3128                                                                                   |
| 701                                                    | 1672                                                | 2512<br>2513                                      | 3280                                           | 788 12134                                                                                  |
| 702                                                    | 1673                                                | 2513                                              | 3280                                           | 788_12134                                                                                  |
| 703                                                    | 1674<br>1675                                        | 2514                                              | 3281                                           | 787 1910                                                                                   |
| 704                                                    | 1676                                                | 2514                                              | 3282                                           | 784 6986                                                                                   |
| 706                                                    | 1677                                                | 2516                                              | 3283                                           | 792 6424                                                                                   |
| 707                                                    | 1678                                                | 2517                                              | 3284                                           | 789 6251                                                                                   |
| 707                                                    | 1679                                                | 2518                                              | 3285                                           | 790 16758                                                                                  |
| 709                                                    | 1680                                                | 2519                                              | 3286                                           | 784 1388                                                                                   |
| 710                                                    | 1681                                                | 2520                                              | 3287                                           | 790 12927                                                                                  |
| 710                                                    | 1682                                                | 2320                                              | 3207                                           | 770_12727                                                                                  |
| 712                                                    | 1683                                                | 2521                                              | 3288                                           | 784 5409                                                                                   |
| 713                                                    | 1684                                                |                                                   | 0200                                           |                                                                                            |
| 714                                                    | 1685                                                | -                                                 |                                                |                                                                                            |
| 715                                                    | 1686                                                | 2522                                              | 3289                                           | 789 6307                                                                                   |
| 716                                                    | 1687                                                | 2523                                              | 3290                                           | 789 6307                                                                                   |
| 717                                                    | 1688                                                | 2524                                              | 3291                                           | 789 5195                                                                                   |
| 718                                                    | 1689                                                | 2525                                              | 3292                                           | 784_3617                                                                                   |
| 719                                                    | 1690                                                | 2526                                              | 3293                                           | 789_4172                                                                                   |
| 720                                                    | 1691                                                | 2527                                              | 3294                                           | 790_15081                                                                                  |
| 721                                                    | 1692                                                | 2528                                              | 3295                                           | 789_4177                                                                                   |
| 722                                                    | 1693                                                | 2529                                              | 3296                                           | 789_2661                                                                                   |
| 723                                                    | 1694                                                | 2530                                              | 3297                                           | 789_1635                                                                                   |
| 724                                                    | 1695                                                | 2531                                              | 3298                                           | 788_8352                                                                                   |
| 725                                                    | 1696                                                | 2532                                              | 3299                                           | 787_9506                                                                                   |
| 726                                                    | 1697                                                | 2533                                              | 3300                                           | 784_7635                                                                                   |
| 727                                                    | 1698                                                | 2534                                              | 3301                                           | 788_9560                                                                                   |
| 728                                                    | 1699                                                | 2535                                              | 3302                                           | 788_12695                                                                                  |
| 729                                                    | 1700                                                | 2536                                              | 3303                                           | 784_691                                                                                    |
| 730                                                    | 1701                                                | 2537                                              | 3304                                           | 784_8513                                                                                   |
| 731                                                    | 1702                                                | 2538                                              | 3305                                           | 784_5838                                                                                   |
| 732                                                    | 1703                                                | 2539                                              | 3306                                           | 784_9765                                                                                   |
| 733                                                    | 1704                                                | 0540                                              | 1                                              | 704 7005                                                                                   |
| 734                                                    | 1705                                                | 2540                                              | 3307                                           | 784_7285                                                                                   |

1142

Table 6

| SEQ ID NO:     | SEQ ID NO:     | SEQ ID NO: | SEQ ID NO:   | Identification of    |
|----------------|----------------|------------|--------------|----------------------|
| of full-length | of full-length | of contig  | of contig    | Priority Application |
| nucleotide     | peptide        | nucleotide | peptide      | that contig          |
| sequence       | sequence       | sequence   | sequence     | nucleotide sequence  |
|                |                |            |              | was filed (Attorney  |
|                |                |            |              | Docket NoSEQ ID      |
|                | 1506           |            |              | NO.) *               |
| 735            | 1706           | 2541       | 2200         | 787 2751             |
| 736            | 1707           | 2541       | 3308<br>3309 | 787 930              |
| 737            | 1708           | 2543       | 3310         | 784 4990             |
| 739            | 1710           | 2544       | 3311         | 784 4990             |
| 740            | 1711           | 2545       | 3312         | 788 9526             |
| 740            | 1712           | 2546       | 3313         | 788 9526             |
| 741            | 1713           | 2547       | 3314         | 788 9526             |
| 743            | 1714           | 2548       | 3315         | 787 3379             |
| 744            | 1715           | 2549       | 3316         | 784 3729             |
| 745            | 1716           | 2550       | 3317         | 789 657              |
| 746            | 1717           | 2551       | 3318         | 784 2162             |
| 747            | 1718           | 2552       | 3319         | 787 3728             |
| 748            | 1719           | 2553       | 3320         | 791 2939             |
| 749            | 1720           | 2554       | 3321         | 787 6837             |
| 750            | 1721           | 2555       | 3322         | 784 5899             |
| 751            | 1722           | 2333       | 0022         |                      |
| 752            | 1723           |            |              |                      |
| 753            | 1724           |            |              |                      |
| 754            | 1725           |            |              |                      |
| 755            | 1726           | 2556       | 3323         | 790 4177             |
| 756            | 1727           |            |              |                      |
| 757            | 1728           | 2557       | 3324         | 784 10284            |
| 758            | 1729           | 2558       | 3325         | 787 2826             |
| 759            | 1730           |            |              |                      |
| 760            | 1731           | 2559       | 3326         | 784 4266             |
| 761            | 1732           | 2560       | 3327         | 790 13065            |
| 762            | 1733           |            |              |                      |
| 763            | 1734           | 2561       | 3328         | 790_3689             |
| 764            | 1735           |            |              |                      |
| 765            | 1736           |            |              |                      |
| 766            | 1737           |            |              |                      |
| 767            | 1738           |            |              |                      |
| 768            | 1739           | 2562       | 3329         | 787_134              |
| 769            | 1740           |            |              |                      |
| 770            | 1741           | 2563       | 3330         | 790_5571             |
| 771            | 1742           | 2564       | 3331         | 790_29586            |
| 772            | 1743           | 2565       | 3332         | 790_795              |
| 773            | 1744           | 2566       | 3333         | 784_9909             |
| 774            | 1745           | 2567       | 3334         | 790_6056             |
| 775            | 1746           | 2568       | 3335         | 787_2295             |
| 776            | 1747           |            |              |                      |
| 777            | 1748           |            |              |                      |
| 778            | 1749           |            |              |                      |
| 779            | 1750           | 2569       | 3336         | 791_1055             |
| 780            | 1751           |            |              |                      |
| 781            | 1752           |            |              |                      |
| 782            | 1753           |            |              |                      |
| 783            | 1754           | 2570       | 3337         | 784_2972             |

1143

Table 6

| SEQ ID NO:     | SEQ ID NO:     | SEQ ID NO:   | SEQ ID NO: | Identification of                          |
|----------------|----------------|--------------|------------|--------------------------------------------|
| of full-length | of full-length | of contig    | of contig  | Priority Application                       |
| nucleotide     | peptide        | nucleotide   | peptide    | that contig                                |
| sequence       | sequence       | sequence     | sequence   | nucleotide sequence<br>was filed (Attorney |
|                |                |              |            | Docket No. SEQ ID                          |
|                |                |              |            | NO.) *                                     |
| 784            | 1755           | 2571         | 3338       | 790 421                                    |
| 785            | 1756           | 2572         | 3339       | 784 9071                                   |
| 786            | 1757           | 2573         | 3340       | 784 9071                                   |
| 787            | 1758           | 2574         | 3341       | 784 2812                                   |
| 788            | 1759           |              |            |                                            |
| 789            | 1760           | 2575         | 3342       | 784 8343                                   |
| 790            | 1761           | 2576         | 3343       | 790 24179                                  |
| 791            | 1762           | 2577         | 3344       | 787_5796                                   |
| 792            | 1763           |              |            |                                            |
| 793            | 1764           |              |            |                                            |
| 794            | 1765           | 2578         | 3345       | 787_2186                                   |
| 795            | 1766           | 2579         | 3346       | 784_3425                                   |
| 796            | 1767           | 2580         | 3347       | 784_2450                                   |
| 797            | 1768           | 2581         | 3348       | 790_10545                                  |
| 798            | 1769           | 2582         | 3349       | 787_10022                                  |
| 799            | 1770           | 2583         | 3350       | 792_7526                                   |
| 800            | 1771           | 2584         | 3351       | 788_6854                                   |
| 801            | 1772           |              |            |                                            |
| 802            | 1773           |              |            |                                            |
| 803            | 1774           |              |            |                                            |
| 804            | 1775           |              |            |                                            |
| 805            | 1776           |              |            |                                            |
| 806            | 1777           | 2585         | 3352       | 790_11591                                  |
| 807            | 1778           |              |            |                                            |
| 808            | 1779           |              |            |                                            |
| 810            | 1780           |              |            |                                            |
| 810            | 1781<br>1782   | 2596         | 22.52      | 700 17405                                  |
| 812            | 1783           | 2586<br>2587 | 3353       | 790_17425<br>787_5611                      |
| 813            | 1784           | 2588         | 3354       | 790 23540                                  |
| 814            | 1785           | 4300         | 3355       | 170_23340                                  |
| 815            | 1786           | 2589         | 3356       | 784 5005                                   |
| 816            | 1787           | 2590         | 3357       | 788 6661                                   |
| 817            | 1788           | 2370         | 3331       | 750_0001                                   |
| 818            | 1789           | 2591         | 3358       | 790 29528                                  |
| 819            | 1790           | 2592         | 3359       | 784 7697                                   |
| 820            | 1791           |              |            | , 31_1071                                  |
| 821            | 1792           |              |            |                                            |
| 822            | 1793           | 2593         | 3360       | 787 3303                                   |
| 823            | 1794           |              |            |                                            |
| 824            | 1795           | 2594         | 3361       | 785 2074                                   |
| 825            | 1796           | 2595         | 3362       | 792 4185                                   |
| 826            | 1797           | -            |            |                                            |
| 827            | 1798           | 2596         | 3363       | 784 3696                                   |
|                |                |              | 3364       |                                            |
| 828            | 1799           | 2597         | 3304       | 784_5320                                   |
| 829            |                | 2597<br>2598 | 3365       | 784_4959                                   |
| 829<br>830     | 1799           |              |            | ·                                          |
| 829            | 1799<br>1800   | 2598         | 3365       | 784_4959                                   |

1144

Table 6

| SEQ ID NO:     | SEQ ID NO:     | SEQ ID NO:   | SEQ ID NO:   | Identification of                          |
|----------------|----------------|--------------|--------------|--------------------------------------------|
| of full-length | of full-length | of contig    | of contig    | Priority Application                       |
| nucleotide     | peptide        | nucleotide   | peptide      | that contig                                |
| sequence       | sequence       | sequence     | sequence     | nucleotide sequence<br>was filed (Attorney |
|                |                |              |              | Docket No. SEQ ID                          |
| · ·            |                |              |              | NO.) *                                     |
| 833            | 1804           |              |              | 1.0.9                                      |
| 834            | 1805           |              |              |                                            |
| 835            | 1806           |              |              |                                            |
| 836            | 1807           | 2602         | 3369         | 788_13648                                  |
| 837            | 1808           |              |              |                                            |
| 838            | 1809           | 2603         | 3370         | 790_17373                                  |
| 839            | 1810           |              |              |                                            |
| 840            | 1811           | 2604         | 3371         | 784_8575                                   |
| 841            | 1812           |              |              |                                            |
| 842            | 1813           | 2605         | 2270         | 797 10047                                  |
| 843            | 1814           | 2605         | 3372         | 787_10247<br>787_3385                      |
| 844            | 1815           | 2606         | 3373         | 101_3363                                   |
| 845<br>846     | 1816<br>1817   |              |              |                                            |
| 847            | 1818           |              |              |                                            |
| 848            | 1819           | 2607         | 3374         | 789 6391                                   |
| 849            | 1820           | 2608         | 3375         | 784 8632                                   |
| 850            | 1821           | 2609         | 3376         | 784 1619                                   |
| 851            | 1822           | 2007         | 30,0         |                                            |
| 852            | 1823           | 2610         | 3377         | 788 8284                                   |
| 853            | 1824           | 2611         | 3378         | 787 1648                                   |
| 854            | 1825           | 2612         | 3379         | 784_8333                                   |
| 855            | 1826           | 2613         | 3380         | 790_13448                                  |
| 856            | 1827           | 2614         | 3381         | 790_27871                                  |
| 857            | 1828           | 2615         | 3382         | 790_11655                                  |
| 858            | 1829           | 2616         | 3383         | 790_17178                                  |
| 859            | 1830           |              |              |                                            |
| 860            | 1831           | 2617         | 3384         | 787_10232                                  |
| 861            | 1832           | 2618         | 3385         | 784_6099                                   |
| 862            | 1833           | 2610         | 2206         | 700 10000                                  |
| 863            | 1834           | 2619         | 3386         | 790_19908                                  |
| 864            | 1835           | 2620         | 3387         | 784_603<br>784_603                         |
| 865            | 1836           | 2621<br>2622 | 3388<br>3389 | 790 27344                                  |
| 866<br>867     | 1837<br>1838   | 2022         | 3309         | 170_41344                                  |
| 868            | 1839           | 2623         | 3390         | 784 10006                                  |
| 869            | 1840           | 2624         | 3391         | 784_10006                                  |
| 870            | 1841           | 2625         | 3392         | 784 10006                                  |
| 871            | 1842           | 2626         | 3393         | 784 10006                                  |
| 872            | 1843           |              |              |                                            |
| 873            | 1844           | 2627         | 3394         | 790_4164                                   |
| 874            | 1845           | 2628         | 3395         | 784_2160                                   |
| 875            | 1846           | 2629         | 3396         | 784_2491                                   |
| 876            | 1847           | 2630         | 3397         | 792_2758                                   |
| 877            | 1848           | 2631         | 3398         | 790_26542                                  |
| 878            | 1849           | 2632         | 3399         | 790_15426                                  |
| 879            | 1850           | 2633         | 3400         | 784_5086                                   |
| 880            | 1851           | 2634         | 3401         | 784_5696                                   |
| 881            | 1852           | 2635         | 3402         | 784_9484                                   |

1145

Table 6

| nucleotide sequence                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        | SEQ ID NO:     | SEQ ID NO:     | SEQ ID NO: | SEQ ID NO: | Identification of    |
|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------|----------------|------------|------------|----------------------|
| sequence         sequence         sequence         sequence was filed (Attorn Docket No. SEQ I NO.) *           882         1853         2636         3403         784 8961           883         1854         884         1855         2637         3404         784 1073           885         1856         2638         3405         787 9241         3866         1857         2639         3406         784 3613           887         1858         2640         3407         784 3481         3481         3481         3481         3481         3481         3481         3481         3481         3481         3481         3481         3481         3481         3481         3481         3481         3481         3481         3481         3481         3481         3481         3481         3481         3481         3481         3481         3481         3481         3481         3481         3481         3481         3481         3481         3481         3481         3481         3481         3481         3481         3481         3481         3481         3481         3481         3481         3481         3481         3481         3481         3481         3481         3481         3481     | of full-length | of full-length | of contig  | of contig  | Priority Application |
| Section                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |                |                | 1          |            |                      |
| 882         1853         2636         3403         784_8961           883         1854         784_8961         884         1855         2637         3404         784_1073           885         1855         2638         3405         787_9241         886         1857         2639         3406         784_3613         3613         887         1858         2640         3407         784_3481         3613         887         1858         2640         3407         784_3481         388         1859         2641         3408         792_1019         199         199         20139         199         1860         2642         3409         790_20139         209         1860         2642         3409         790_20139         209         1861         2643         3410         784_7697         3891         1862         2644         3411         790_669         3891         1862         2644         3411         790_669         3892         1863         3412         784_9086         3893         1864         3412         784_9086         3895         1866         2645         3412         784_9086         3895         1866         2646         3413         785_610         3896         1867 | sequence       | sequence       | sequence   | sequence   |                      |
| 882         1853         2636         3403         784_8961           883         1854                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |                |                |            |            |                      |
| 882         1853         2636         3403         784_8961           883         1854                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |                |                |            |            |                      |
| 883         1854         3404         784 1073           884         1855         2638         3405         787 9241           885         1856         2638         3405         787 9241           886         1857         2639         3406         784 3613           887         1858         2640         3407         784 3481           888         1859         2641         3408         792 1019           889         1860         2642         3409         790 20139           890         1861         2643         3410         784 7697           891         1862         2644         3411         790 669           892         1863         893         1864         894           894         1865         2645         3412         784 9086           895         1866         2646         3413         785 610           896         1867         2647         3414         784 9086           898         1869         2649         3416         789 350           899         1870         2650         3417         784 221           900         1871         902         1873                                                                                                                              | 000            | 1052           | 2626       | 3403       |                      |
| 884         1855         2637         3404         784         1073           885         1856         2638         3405         787         9241           886         1857         2639         3406         784         3613           887         1858         2640         3407         784         3481           888         1859         2641         3408         792         1019           889         1860         2642         3409         790         20139           890         1861         2643         3410         784         7697           891         1862         2644         3411         790         669           892         1863                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |                |                | 2030       | 3403       | 701 0201             |
| 885         1856         2638         3405         787 9241           886         1857         2639         3406         784 3613           887         1858         2640         3407         784 3481           888         1859         2641         3408         792 1019           889         1860         2642         3409         790 20139           890         1861         2643         3410         784 7697           891         1862         2644         3411         790 669           892         1863                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |                |                | 2637       | 3404       | 784 1073             |
| 886         1857         2639         3406         784_3613           887         1858         2640         3407         784_3481           888         1859         2641         3408         792_1019           889         1860         2642         3409         790_20139           889         1861         2643         3410         784_7697           891         1862         2644         3411         790_669           892         1863                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |                |                |            |            |                      |
| 887         1858         2640         3407         784_3481           888         1859         2641         3408         792_1019           889         1860         2642         3409         790_20139           890         1861         2643         3410         784_7697           891         1862         2644         3411         790_669           892         1863                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |                |                |            |            | 784 3613             |
| 888         1859         2641         3408         792_1019           889         1860         2642         3409         790_20139           890         1861         2643         3410         784_7697           891         1862         2644         3411         790_669           892         1863                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |                |                |            |            |                      |
| 889         1860         2642         3409         790_20139           890         1861         2643         3410         784_7697           891         1862         2644         3411         790_669           892         1863                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |                |                |            |            | 792 1019             |
| 890         1861         2643         3410         784_7697           891         1862         2644         3411         790_669           892         1863                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |                |                |            |            |                      |
| 891         1862         2644         3411         790 669           892         1863                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |                |                |            |            | 784 7697             |
| 892         1863           893         1864           894         1865         2645         3412         784 9086           895         1866         2646         3413         785 610           896         1867         2647         3414         784 382           897         1868         2648         3415         790 436           898         1869         2649         3416         789 350           899         1870         2650         3417         784 221           900         1871                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |                |                |            |            | 790 669              |
| 893         1864           894         1865         2645         3412         784_9086           895         1866         2646         3413         785_610           896         1867         2647         3414         784_382           897         1868         2648         3415         790_436           898         1869         2649         3416         789_350           899         1870         2650         3417         784_221           900         1871                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |                |                |            |            |                      |
| 894         1865         2645         3412         784_9086           895         1866         2646         3413         785_610           896         1867         2647         3414         784_382           897         1868         2648         3415         790_436           898         1869         2649         3416         789_350           899         1870         2650         3417         784_221           900         1871                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |                |                |            |            |                      |
| 895         1866         2646         3413         785_610           896         1867         2647         3414         784_382           897         1868         2648         3415         790_436           898         1869         2649         3416         789_350           899         1870         2650         3417         784_221           900         1871                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |                |                | 2645       | 3412       | 784_9086             |
| 896         1867         2647         3414         784 382           897         1868         2648         3415         790 436           898         1869         2649         3416         789 350           899         1870         2650         3417         784 221           900         1871                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |                |                |            |            |                      |
| 897         1868         2648         3415         790_436           898         1869         2649         3416         789_350           899         1870         2650         3417         784_221           900         1871                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |                |                |            |            | 784 382              |
| 898         1869         2649         3416         789 350           899         1870         2650         3417         784 221           900         1871                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |                |                |            |            | 790 436              |
| 899         1870         2650         3417         784_221           900         1871                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |                |                |            |            | 789 350              |
| 900         1871         901         1872           902         1873         2651         3418         784         1121           903         1874         2652         3419         784         3651           904         1875         2653         3420         784         1084           905         1876         2654         3421         784         3935           906         1877         2655         3422         784         7140           907         1878         2656         3423         784         4580           908         1879         2657         3424         790         12684           909         1880         2658         3425         784         9819           910         1881         2659         3426         784         454           911         1882         2660         3427         791         3463           912         1883         2661         3428         790         13539           913         1884         2662         3429         790         85           914         1885         2663         3430         790         29490                                                                                                                                            |                |                |            | 3417       | 784 221              |
| 901         1872           902         1873         2651         3418         784 1121           903         1874         2652         3419         784 3651           904         1875         2653         3420         784 1084           905         1876         2654         3421         784 3935           906         1877         2655         3422         784 7140           907         1878         2656         3423         784 4580           908         1879         2657         3424         790 12684           909         1880         2658         3425         784 9819           910         1881         2659         3426         784 454           911         1882         2660         3427         791 3463           912         1883         2661         3428         790 13539           913         1884         2662         3429         790 85           914         1885         2663         3430         790 29490           915         1886         2664         3431         787 2532           916         1887         2665         3432         791 2376                                                                                                                                 |                |                |            |            |                      |
| 902         1873         2651         3418         784 1121           903         1874         2652         3419         784 3651           904         1875         2653         3420         784 1084           905         1876         2654         3421         784 3935           906         1877         2655         3422         784 7140           907         1878         2656         3423         784 4580           908         1879         2657         3424         790 12684           909         1880         2658         3425         784 9819           910         1881         2659         3426         784 454           911         1882         2660         3427         791 3463           912         1883         2661         3428         790 13539           913         1884         2662         3429         790 85           914         1885         2663         3430         790 29490           915         1886         2664         3431         787 2532           916         1887         2665         3432         791 2376           917         1888                                                                                                                                 |                |                |            |            |                      |
| 903         1874         2652         3419         784 3651           904         1875         2653         3420         784 1084           905         1876         2654         3421         784 3935           906         1877         2655         3422         784 7140           907         1878         2656         3423         784 4580           908         1879         2657         3424         790 12684           909         1880         2658         3425         784 9819           910         1881         2659         3426         784 454           911         1882         2660         3427         791 3463           912         1883         2661         3428         790 13539           913         1884         2662         3429         790 85           914         1885         2663         3430         790 29490           915         1886         2664         3431         787 2532           916         1887         2665         3432         791 2376           917         1888         2666         3433         784 1870           918         1889                                                                                                                                 |                |                | 2651       | 3418       | 784 1121             |
| 904         1875         2653         3420         784 1084           905         1876         2654         3421         784 3935           906         1877         2655         3422         784 7140           907         1878         2656         3423         784 4580           908         1879         2657         3424         790 12684           909         1880         2658         3425         784 9819           910         1881         2659         3426         784 454           911         1882         2660         3427         791 3463           912         1883         2661         3428         790 13539           913         1884         2662         3429         790 85           914         1885         2663         3430         790 29490           915         1886         2664         3431         787 2532           916         1887         2665         3432         791 2376           917         1888         2666         3433         784 1870           918         1889         2667         3434         784 9111                                                                                                                                                            |                |                |            |            | 784 3651             |
| 905         1876         2654         3421         784 3935           906         1877         2655         3422         784 7140           907         1878         2656         3423         784 4580           908         1879         2657         3424         790 12684           909         1880         2658         3425         784 9819           910         1881         2659         3426         784 454           911         1882         2660         3427         791 3463           912         1883         2661         3428         790 13539           913         1884         2662         3429         790 85           914         1885         2663         3430         790 29490           915         1886         2664         3431         787 2532           916         1887         2665         3432         791 2376           917         1888         2666         3433         784 1870           918         1889         2667         3434         784 9111                                                                                                                                                                                                                                  |                |                |            | 3420       | 784 1084             |
| 906         1877         2655         3422         784 7140           907         1878         2656         3423         784 4580           908         1879         2657         3424         790 12684           909         1880         2658         3425         784 9819           910         1881         2659         3426         784 454           911         1882         2660         3427         791 3463           912         1883         2661         3428         790 13539           913         1884         2662         3429         790 85           914         1885         2663         3430         790 29490           915         1886         2664         3431         787 2532           916         1887         2665         3432         791 2376           917         1888         2666         3433         784 1870           918         1889         2667         3434         784 9111                                                                                                                                                                                                                                                                                                        |                |                |            | 3421       | 784_3935             |
| 907         1878         2656         3423         784 4580           908         1879         2657         3424         790 12684           909         1880         2658         3425         784 9819           910         1881         2659         3426         784 454           911         1882         2660         3427         791 3463           912         1883         2661         3428         790 13539           913         1884         2662         3429         790 85           914         1885         2663         3430         790 29490           915         1886         2664         3431         787 2532           916         1887         2665         3432         791 2376           917         1888         2666         3433         784 1870           918         1889         2667         3434         784 9111                                                                                                                                                                                                                                                                                                                                                                              |                |                |            | 3422       |                      |
| 908         1879         2657         3424         790_12684           909         1880         2658         3425         784_9819           910         1881         2659         3426         784_454           911         1882         2660         3427         791_3463           912         1883         2661         3428         790_13539           913         1884         2662         3429         790_85           914         1885         2663         3430         790_29490           915         1886         2664         3431         787_2532           916         1887         2665         3432         791_2376           917         1888         2666         3433         784_1870           918         1889         2667         3434         784_9111                                                                                                                                                                                                                                                                                                                                                                                                                                                    |                |                |            | 3423       | 784_4580             |
| 910         1881         2659         3426         784 454           911         1882         2660         3427         791 3463           912         1883         2661         3428         790 13539           913         1884         2662         3429         790 85           914         1885         2663         3430         790 29490           915         1886         2664         3431         787 2532           916         1887         2665         3432         791 2376           917         1888         2666         3433         784 1870           918         1889         2667         3434         784 9111                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |                |                | 2657       | 3424       | 790_12684            |
| 911         1882         2660         3427         791 3463           912         1883         2661         3428         790 13539           913         1884         2662         3429         790 85           914         1885         2663         3430         790 29490           915         1886         2664         3431         787 2532           916         1887         2665         3432         791 2376           917         1888         2666         3433         784 1870           918         1889         2667         3434         784 9111                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      | 909            | 1880           | 2658       | 3425       | 784_9819             |
| 912         1883         2661         3428         790 13539           913         1884         2662         3429         790 85           914         1885         2663         3430         790 29490           915         1886         2664         3431         787 2532           916         1887         2665         3432         791 2376           917         1888         2666         3433         784 1870           918         1889         2667         3434         784 9111                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            | 910            | 1881           | 2659       | 3426       | 784_454              |
| 913         1884         2662         3429         790 85           914         1885         2663         3430         790 29490           915         1886         2664         3431         787 2532           916         1887         2665         3432         791 2376           917         1888         2666         3433         784 1870           918         1889         2667         3434         784 9111                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | 911            | 1882           | 2660       | 3427       |                      |
| 914         1885         2663         3430         790 29490           915         1886         2664         3431         787 2532           916         1887         2665         3432         791 2376           917         1888         2666         3433         784 1870           918         1889         2667         3434         784 9111                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       | 912            | 1883           | 2661       | 3428       |                      |
| 915         1886         2664         3431         787 2532           916         1887         2665         3432         791 2376           917         1888         2666         3433         784 1870           918         1889         2667         3434         784 9111                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              | 913            | 1884           | 2662       |            |                      |
| 915     1886     2664     3431     787 2532       916     1887     2665     3432     791 2376       917     1888     2666     3433     784 1870       918     1889     2667     3434     784 9111                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |                | 1005           | 2663       | 3430       | 790_29490            |
| 916     1887     2665     3432     791 2376       917     1888     2666     3433     784 1870       918     1889     2667     3434     784 9111                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            | 915            |                | 2664       |            |                      |
| 917     1888     2666     3433     784 1870       918     1889     2667     3434     784 9111                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |                |                |            |            |                      |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |                | 1888           |            |            |                      |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            | 918            | 1889           | 2667       |            |                      |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            | 919            | 1890           | 2668       | 3435       | 784_2245             |
| 920 1891 2669 3436 784_9212                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | 920            | 1891           |            |            |                      |
| 921 1892 2670 3437 784 2900                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | 921            |                | 2670       | 3437       | 784_2900             |
| 922 1893                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |                |                |            |            |                      |
| 923 1894                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | 923            |                |            |            |                      |
| 924         1895         2671         3438         787_3438                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |                |                |            |            |                      |
| 925 1896 2672 3439 787_4767                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |                | 1896           |            |            |                      |
| 926         1897         2673         3440         787_4767                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | 926            |                |            |            |                      |
| 927 1898 2674 3441 787_2408                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | 927            |                |            |            |                      |
| 928 1899 2675 3442 791_311                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 | 928            |                | 2675       | 3442       | 791_311              |
| 929 1900                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |                |                |            |            |                      |
| 930 1901                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | 930            | 1901           | <u></u>    |            |                      |

1146

Table 6

| SEQ ID NO:<br>of full-length<br>nucleotide | SEQ ID NO:<br>of full-length<br>peptide | SEQ ID NO:<br>of contig<br>nucleotide | SEQ ID NO:<br>of contig<br>peptide | Identification of Priority Application that contig        |
|--------------------------------------------|-----------------------------------------|---------------------------------------|------------------------------------|-----------------------------------------------------------|
| sequence                                   | sequence                                | sequence                              | sequence                           | nucleotide sequence was filed (Attorney Docket No. SEQ ID |
|                                            |                                         |                                       |                                    | NO.) *                                                    |
| 931                                        | 1902                                    | 2676                                  | 3443                               | 787 233                                                   |
| 932                                        | 1903                                    |                                       | 114.00                             |                                                           |
| 933                                        | 1904                                    | 2677                                  | 3444                               | 787 4124                                                  |
| 934                                        | 1905                                    | 2678                                  | 3445                               | 787_4124                                                  |
| 935                                        | 1906                                    | 2679                                  | 3446                               | 791_1604                                                  |
| 936                                        | 1907                                    |                                       |                                    |                                                           |
| 937                                        | 1908                                    | 2680                                  | 3447                               | 784_1468                                                  |
| 938                                        | 1909                                    | 2681                                  | 3448                               | 787_1602                                                  |
| 939                                        | 1910                                    | 2682                                  | 3449                               | 784_6971                                                  |
| 940                                        | 1911                                    | 2683                                  | 3450                               | 784_9131                                                  |
| 941                                        | 1912                                    | 2684                                  | 3451                               | 788_1717                                                  |
| 942                                        | 1913                                    | 2685                                  | 3452                               | 787_2644                                                  |
| 943                                        | 1914                                    | 2686                                  | 3453                               | 784_4755                                                  |
| 944                                        | 1915                                    | 2687                                  | 3454                               | 784_5576                                                  |
| 945                                        | 1916                                    | 2688                                  | 3455                               | 784_5576                                                  |
| 946                                        | 1917                                    | 2689                                  | 3456                               | 787_8607                                                  |
| 947                                        | 1918                                    |                                       |                                    |                                                           |
| 948                                        | 1919                                    |                                       |                                    |                                                           |
| 949                                        | 1920                                    | 2690                                  | 3457                               | 784_3786                                                  |
| 950                                        | 1921                                    | 2691                                  | 3458                               | 790_6872                                                  |
| 951                                        | 1922                                    | 2692                                  | 3459                               | 784_5341                                                  |
| 952                                        | 1923                                    | 2693                                  | 3460                               | 788_7215                                                  |
| 953                                        | 1924                                    | 2694                                  | 3461                               | 790_23518                                                 |
| 954                                        | 1925                                    | 2695                                  | 3462                               | 784 668                                                   |
| 955                                        | 1926                                    | 2696                                  | 3463                               | 787 7442                                                  |
| 956                                        | 1927                                    | 2697                                  | 3464                               | 784 2563                                                  |
| 957                                        | 1928                                    | 2698                                  | 3465                               | 784_10090                                                 |
| 958                                        | 1929                                    | 2699                                  | 3466                               | 787_1110                                                  |
| 959                                        | 1930                                    | 2700                                  | 3467                               | 784_2417                                                  |
| 960                                        | 1931                                    |                                       |                                    |                                                           |
| 961                                        | 1932                                    | 2701                                  | 3468                               | 784_1346                                                  |
| 962                                        | 1933                                    | 2702                                  | 3469                               | 784_2272                                                  |
| 963                                        | 1934                                    | 2703                                  | 3470                               | 784_4173                                                  |
| 964                                        | 1935                                    | 2704                                  | 3471                               | 784_9318                                                  |
| 965                                        | 1936                                    | 2705                                  | 3472                               | 784_5363                                                  |
| 966                                        | 1937                                    | 2706                                  | 3473                               | 784_4084                                                  |
| 967                                        | 1938                                    |                                       |                                    |                                                           |
| 968                                        | 1939                                    |                                       |                                    |                                                           |
| 969                                        | 1940                                    | 2707                                  | 3474                               | 790 4256                                                  |
| 970                                        | 1941                                    | 2708                                  | 3475                               | 784_446                                                   |
| 971                                        | 1942                                    | 2709                                  | 3476                               | 790 11491                                                 |

<sup>\*784</sup>\_XXX = SEQ ID NO: XXX of Attorney Docket No. 784, US Serial No. 09/488,725 filed 01/21/2000, the entire disclosure of which, including sequence listing, is incorporated herein by reference.

<sup>785</sup>\_XXX = SEQ ID NO: XXX of Attorney Docket No. 785, US Serial No. 09/491,404 filed 01/25/2000, the entire disclosure of which, including sequence listing, is incorporated herein by reference.

## 1147

## Table 6

787\_XXX = SEQ ID NO: XXX of Attorney Docket No. 787, US Serial No. 09/496,914 filed 02/03/2000, the entire disclosure of which, including sequence listing, is incorporated herein by reference.

788\_XXX = SEQ ID NO: XXX of Attorney Docket No. 788, US Serial No. 09/515,126 filed 02/28/2000, the entire disclosure of which, including sequence listing, is incorporated herein by reference.

789\_XXX = SEQ ID NO: XXX of Attorney Docket No. 789, US Serial No. 09/519,705 filed 03/07/2000, the entire disclosure of which, including sequence listing, is incorporated herein by reference.

790\_XXX = SEQ ID NO: XXX of Attorney Docket No. 790, US Serial No. 09/540,217 filed 03/31/2000, the entire disclosure of which, including sequence listing, is incorporated herein by reference.

791\_XXX = SEQ ID NO: XXX of Attorney Docket No. 791, US Serial No. 09/552,929 filed 04/18/2000, the entire disclosure of which, including sequence listing, is incorporated herein by reference.

792\_XXX = SEQ ID NO: XXX of Attorney Docket No. 792, US Serial No. 09/577,408 filed 05/18/2000, the entire disclosure of which, including sequence listing, is incorporated herein by reference.

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Table 7

| Table 7 |                     |  |  |  |
|---------|---------------------|--|--|--|
| SEQ ID  | Chromsomal location |  |  |  |
| 1       | 16                  |  |  |  |
| 3       | 6q23                |  |  |  |
| 3       | 6q23                |  |  |  |
| 4       | 6q23                |  |  |  |
| 5<br>6  | 7q31<br>5           |  |  |  |
| 6       | 5                   |  |  |  |
| 7       | 11q12               |  |  |  |
| 8       | 4                   |  |  |  |
| 9       | 4                   |  |  |  |
| 10      | 1                   |  |  |  |
| 11      | 18                  |  |  |  |
| 12      | 15q26               |  |  |  |
| 13      | 14                  |  |  |  |
| 14      | 12                  |  |  |  |
| 15      | 5                   |  |  |  |
| 16      | Xp11.1-11.3         |  |  |  |
| 17      | 11q14               |  |  |  |
| 18      | 6q21.               |  |  |  |
| 18      |                     |  |  |  |
| 19      | 11<br>16            |  |  |  |
| 20      |                     |  |  |  |
| 23      | 16                  |  |  |  |
| 24      | 10q24-q25           |  |  |  |
| 25      | 18                  |  |  |  |
| 26      | 17                  |  |  |  |
| 27      | Xp11.21-11.3.       |  |  |  |
| 28      | 16                  |  |  |  |
| 29      | 8                   |  |  |  |
| 30      | 10                  |  |  |  |
| 31      | 6                   |  |  |  |
| 32      | 12                  |  |  |  |
| 33      | 3p24.3              |  |  |  |
| 34      | 17                  |  |  |  |
| 35      | 17                  |  |  |  |
| 36      | 4                   |  |  |  |
| 38      | 1p32.2-34.2         |  |  |  |
| 39      | 9                   |  |  |  |
| 40      | 10                  |  |  |  |
| 41      | 17                  |  |  |  |
| 42      | 1                   |  |  |  |
| 43      | 20p11.23-20p11.22   |  |  |  |
| 44      | 2                   |  |  |  |
| 47      | 2                   |  |  |  |
| 48      | 21                  |  |  |  |
| 40      | 20                  |  |  |  |
| 49      | 3                   |  |  |  |
| 50      |                     |  |  |  |
| 51      | 14                  |  |  |  |
| 52      | 6p21.2-21.31.       |  |  |  |
| 54      | 19                  |  |  |  |
| 55      | 15q11.1             |  |  |  |
| 56      | 12pter-p13.31       |  |  |  |
| 57      | 12pter-p13.31       |  |  |  |
| 58      | 20                  |  |  |  |
| 59      | 17q24-q25           |  |  |  |
| 60      | 9                   |  |  |  |
| 61      | 17                  |  |  |  |
| ···     |                     |  |  |  |

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Table 7

| Table 7 |                     |  |  |  |
|---------|---------------------|--|--|--|
| SEQ ID  | Chromsomal location |  |  |  |
| 62      | 6q14.3-16.2         |  |  |  |
| 63      | 17                  |  |  |  |
| 64      | 16                  |  |  |  |
| 65      | 12p13               |  |  |  |
| 66      | 1p36.11-36.2.       |  |  |  |
| 67      | 6q23                |  |  |  |
| 70      | 19q13.4             |  |  |  |
| 71      | 9q32-33.2           |  |  |  |
| 72      | 6p12.2              |  |  |  |
| 72      | Op12.2              |  |  |  |
| 73      | 6p12.2              |  |  |  |
| 74      | 6p12.2              |  |  |  |
| 76      | 15q15.3             |  |  |  |
| 77      | 20                  |  |  |  |
| 79      | 11pter-p15.5        |  |  |  |
| 80      | 9                   |  |  |  |
| 81      | 2q37                |  |  |  |
| 83      | 4                   |  |  |  |
| 84      | 8                   |  |  |  |
| 85      | 17                  |  |  |  |
| 86      | 16                  |  |  |  |
| 87      | 5p15.2-q12.3        |  |  |  |
| 90      | 19                  |  |  |  |
| 91      | 20                  |  |  |  |
| 92      | 13                  |  |  |  |
| 94      | 17                  |  |  |  |
| 95      | 12                  |  |  |  |
| 96      | 6q14.2-16.1         |  |  |  |
| 97      | 18                  |  |  |  |
| 98      | 15q21.3             |  |  |  |
| 99      | 17                  |  |  |  |
| 100     | 2                   |  |  |  |
|         | 17                  |  |  |  |
| 101     | 19                  |  |  |  |
| 102     | 6                   |  |  |  |
| 103     |                     |  |  |  |
| 104     | 7q36                |  |  |  |
| 105     | 20.                 |  |  |  |
| 106     | 4                   |  |  |  |
| 108     | 11q13               |  |  |  |
| 109     | 16                  |  |  |  |
| 110     | 19                  |  |  |  |
| 111     | 3                   |  |  |  |
| 114     | 19                  |  |  |  |
| 115     | 17                  |  |  |  |
| 116     | 16                  |  |  |  |
| 117     | 19                  |  |  |  |
| 118     | 5                   |  |  |  |
| 122     | 6p12.3-21.2         |  |  |  |
| 123     | 9                   |  |  |  |
| 124     | 3                   |  |  |  |
| 126     | 1q21.2-q22          |  |  |  |
| 127     | 11                  |  |  |  |
| 128     | 15                  |  |  |  |
| 129     | 15                  |  |  |  |
| 130     | 6p12.2-21.1         |  |  |  |
| 131     | 2                   |  |  |  |
|         |                     |  |  |  |

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Table 7

| Table 7 |                     |  |  |  |
|---------|---------------------|--|--|--|
| SEQ ID  | Chromsomal location |  |  |  |
| 132     | 10                  |  |  |  |
| 135     | 20q11.2-q12         |  |  |  |
| 136     | 20q11.2-q12         |  |  |  |
| 137     | 18q11               |  |  |  |
| 138     | 11q22.3-q23         |  |  |  |
| 140     | 2p23.3-q34          |  |  |  |
| 142     | 19                  |  |  |  |
| 143     | 15                  |  |  |  |
|         | 8                   |  |  |  |
| 144     | 16q24.1             |  |  |  |
| 145     | 17                  |  |  |  |
| 146     |                     |  |  |  |
| 149     | 16                  |  |  |  |
| 150     | 10                  |  |  |  |
| 151     | 17                  |  |  |  |
| 152     | 19                  |  |  |  |
| 153     | 16p12               |  |  |  |
| 157     | 20p11.21-11.23.     |  |  |  |
| 159     | 13                  |  |  |  |
| 160     | 13                  |  |  |  |
| 163     | 5                   |  |  |  |
| 164     | X                   |  |  |  |
| 165     | 11                  |  |  |  |
| 166     | 9                   |  |  |  |
| 167     | 1                   |  |  |  |
| 169     | 1                   |  |  |  |
| 170     | 17                  |  |  |  |
| 171     | 6p21.3              |  |  |  |
| 172     | 15q13               |  |  |  |
| 173     | 17                  |  |  |  |
| 173     | 3                   |  |  |  |
| 175     | 12                  |  |  |  |
| 175     | 19p13.2             |  |  |  |
| 177     | 5                   |  |  |  |
| 179     | 9                   |  |  |  |
| 180     |                     |  |  |  |
| 181     | 17                  |  |  |  |
| 182     | 22q13.1-13.2        |  |  |  |
| 184     | 17                  |  |  |  |
| 185     | 15                  |  |  |  |
| 186     | 3                   |  |  |  |
| 187     | 8q24-qter           |  |  |  |
| 188     | 3                   |  |  |  |
| 189     | 4q22-q24            |  |  |  |
| 190     | 19                  |  |  |  |
| 191     | 18p11.3             |  |  |  |
| 192     | 19                  |  |  |  |
| 193     | 11                  |  |  |  |
| 195     | 4                   |  |  |  |
| 196     | 6                   |  |  |  |
| 198     | 19                  |  |  |  |
| 199     | 4                   |  |  |  |
| 200     | Xq28                |  |  |  |
| 200     | 19                  |  |  |  |
|         | 2                   |  |  |  |
| 203     | 19                  |  |  |  |
| 205     |                     |  |  |  |
| 207     | 17                  |  |  |  |

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Table 7

| Table 7    |                     |  |  |  |
|------------|---------------------|--|--|--|
| SEQ ID     | Chromsomal location |  |  |  |
| 208        | 15                  |  |  |  |
| 209        | 1p36.11-36.23       |  |  |  |
| 214        | 2                   |  |  |  |
| 215        | 3                   |  |  |  |
| 216        | 3                   |  |  |  |
| 217        | 22q13.1.            |  |  |  |
| 218        | 12                  |  |  |  |
| 219        | 14                  |  |  |  |
| 220        | 9q34.1              |  |  |  |
| 222        | 17q21               |  |  |  |
| 223        | 19                  |  |  |  |
| 224        | 8                   |  |  |  |
| 225        | 18                  |  |  |  |
| 226        | 1                   |  |  |  |
| 228        | 11q                 |  |  |  |
| 229        | 4                   |  |  |  |
| 230        | 8                   |  |  |  |
| 231        | 6                   |  |  |  |
| 235        | 19                  |  |  |  |
| 236        | 4                   |  |  |  |
| 237        | 20                  |  |  |  |
| 238        | 17                  |  |  |  |
| 239        | 5                   |  |  |  |
| 240        | 5                   |  |  |  |
| 243        | 19                  |  |  |  |
| 244        | 11                  |  |  |  |
|            | 3                   |  |  |  |
| 246<br>247 | 10                  |  |  |  |
| 248        | 5                   |  |  |  |
| 240        | 11                  |  |  |  |
| 249        | 19                  |  |  |  |
| 250        | 15                  |  |  |  |
| 251<br>253 | 4                   |  |  |  |
|            | 18                  |  |  |  |
| 254        | 9                   |  |  |  |
| 255        | 9                   |  |  |  |
| 256        | 11                  |  |  |  |
| 257        | 1                   |  |  |  |
| 258        |                     |  |  |  |
| 259        | 10                  |  |  |  |
| 261<br>262 | 6                   |  |  |  |
| 264        | 5p14.3-q15          |  |  |  |
|            | 6                   |  |  |  |
| 268        |                     |  |  |  |
| 269        | 18p11.3<br>8        |  |  |  |
| 270        |                     |  |  |  |
| 271        | 1q42.11-42.3        |  |  |  |
| 272        | 3                   |  |  |  |
| 273        | 2                   |  |  |  |
| 275        | X                   |  |  |  |
| 276        | 15                  |  |  |  |
| 278        | 3                   |  |  |  |
| 279        | X                   |  |  |  |
| 280        | 7q33                |  |  |  |
| 282        | 3                   |  |  |  |
| 283        | 3                   |  |  |  |

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Table 7

| SEQ ID        | Table 7  Chromsomal location |
|---------------|------------------------------|
| 284           | 15                           |
|               | 7                            |
| 286           | 5                            |
| 287           |                              |
| 288           | 9q34.11-34.13                |
| 290           | 15                           |
| 291           | 14q21                        |
| 292           | 15q21.3                      |
| 293           | 19                           |
| 294           | 16                           |
| 296           | 12                           |
| 297           | 19                           |
| 298           | 14q24.3                      |
| 299           | 20p11                        |
| 300           | 18p11.2                      |
| 00001262Fb231 |                              |
| 301           | 3                            |
| 304           | 9p12-13.3                    |
| 305           | 17                           |
|               | 6                            |
| 306           | 20                           |
| 308           |                              |
| 309           | 16                           |
| 310           | 18                           |
| 311           | 4q26-q27                     |
| 312           | 5                            |
| 314           | 8p23                         |
| 315           | 11                           |
| 316           | 3                            |
| 317           | 3                            |
| 318           | 1q22-q23                     |
| 319           | 22q12.3-13.2                 |
| 320           | 13q12.11-12.3                |
| 321           | 7                            |
| 323           | 11                           |
| 324           | 18                           |
| 325           | 1                            |
| 327           | 6q22.1-6q22.33               |
| 328           | 9                            |
| 329           | 5                            |
|               |                              |
| 331           | 5 8                          |
| 332           |                              |
| 334           | 12q                          |
| 336           | 9                            |
| 337           | 19                           |
| 338           | 5                            |
| 339           | 15                           |
| 340           | 3q                           |
| 341           | 13                           |
| 342           | 18                           |
| 343           | 1p31.2-32.2                  |
| 344           | 2                            |
| 345           | 17                           |
| 346           | 11q14                        |
| 347           | 19q13.13-q13.2               |
| 348           | 19                           |
|               | 3                            |
| 349           |                              |

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Table 7

| SEO ID Chromsomal location |                    |  |  |
|----------------------------|--------------------|--|--|
| SEQ ID                     |                    |  |  |
| 350                        | 17                 |  |  |
| 351                        |                    |  |  |
| 352                        | 19q13.4            |  |  |
| 353                        | 8q                 |  |  |
| 354                        | 14                 |  |  |
| 356                        | 16                 |  |  |
| 357                        | 18q12              |  |  |
| 358                        | 17q11              |  |  |
| 359                        | Xp11.1-11.3        |  |  |
| 360                        | 4                  |  |  |
| 362                        | 19                 |  |  |
| 363                        | 17                 |  |  |
| 364                        | 11q22              |  |  |
| 365                        | 19                 |  |  |
| 366                        | 15                 |  |  |
| 367                        | 5                  |  |  |
| 369                        | 21q22.2D21S349-MX1 |  |  |
| 370                        | 8                  |  |  |
| 371                        | 3p                 |  |  |
| 373                        | 19                 |  |  |
| 374                        | 8q24.1-q24.2       |  |  |
| 375                        | 16                 |  |  |
| 377                        | 17                 |  |  |
| 378                        | 16                 |  |  |
| 380                        | 17                 |  |  |
| 381                        | 1                  |  |  |
| 382                        | 16                 |  |  |
| 383                        | 19                 |  |  |
| 384                        | Xq22.1-23          |  |  |
| 385                        | 5p                 |  |  |
| 386                        | X                  |  |  |
| 387                        | 19                 |  |  |
| 388                        | 4p16               |  |  |
| 389                        | 8                  |  |  |
| 391                        | 21q22.3            |  |  |
| 392                        | 11                 |  |  |
| 393                        | 19                 |  |  |
| 396                        | 19                 |  |  |
| 398                        | 19                 |  |  |
| 400                        | 1q32               |  |  |
| 402                        | 13q34              |  |  |
| 403                        | X                  |  |  |
| 404                        | 16                 |  |  |
| 406                        | 5                  |  |  |
| 407                        | 18                 |  |  |
| 409                        | 3                  |  |  |
| 410                        | 1                  |  |  |
| 411                        | 1                  |  |  |
| 412                        | 1                  |  |  |
| 413                        | 7                  |  |  |
| 414                        | 19q13.3-q13.4      |  |  |
| 415                        | 6                  |  |  |
| 416                        | 9                  |  |  |
| 417                        | 14                 |  |  |
| 418                        | 1                  |  |  |
| _ T_1O                     |                    |  |  |

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Table 7

| Table 7  SEO ID Chromsomal location |               |  |
|-------------------------------------|---------------|--|
| SEQ ID                              |               |  |
| 419                                 | 5             |  |
| 421                                 |               |  |
| 422                                 | 02            |  |
| 423                                 | 8p22          |  |
| 424                                 | 11            |  |
| 425                                 | 6q12-13       |  |
| 426                                 | 19q13.43      |  |
| 427                                 | X             |  |
| 428                                 | 6             |  |
| 429                                 | 5             |  |
| 430                                 | 20            |  |
| 00001814Fc201                       |               |  |
| 431                                 | 11            |  |
| 433                                 | 19            |  |
| 434                                 | 12q           |  |
| 436                                 | 4q28          |  |
| 437                                 | 15            |  |
|                                     | 12            |  |
| 438                                 | 1             |  |
| 440                                 |               |  |
| 441                                 | 5q            |  |
| 442                                 | 6p12.3-21.2   |  |
| 443                                 | 7q35          |  |
| 446                                 | 11q13         |  |
| 447                                 | X             |  |
| 448                                 | X             |  |
| 449                                 | 14q24.3       |  |
| 452                                 | 17q12-q21     |  |
| 455                                 | 17            |  |
| 456                                 | 4             |  |
| 457                                 | 7             |  |
| 459                                 | 18q11.2       |  |
| 463                                 | 5             |  |
| 464                                 | 22q12         |  |
| 465                                 | 5             |  |
| 467                                 | 15            |  |
| 468                                 | 19            |  |
|                                     | 2             |  |
| 469                                 |               |  |
| 471                                 | 20            |  |
| 473                                 | unknown       |  |
| 474                                 | 17            |  |
| 475                                 | 2             |  |
| 476                                 | 17            |  |
| 477                                 | 17            |  |
| 478                                 | 20p12.3-13.   |  |
| 479                                 | 17            |  |
| 480                                 | 19            |  |
| 481                                 | 20            |  |
| 483                                 | 19            |  |
| 486                                 | 15q15         |  |
| 487                                 | 10p12.1-p11.1 |  |
| 490                                 | 5q35          |  |
| 491                                 | 19            |  |
| 491                                 |               |  |
|                                     | 16p13.3       |  |
| 493                                 | 16p13.3       |  |
| 494                                 | 17            |  |

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Table 7

| Table 7       |                     |  |
|---------------|---------------------|--|
| SEQ ID        | Chromsomal location |  |
| 495           | 8                   |  |
| 496           | 3                   |  |
| 497           | 11q23               |  |
| 498           | 3                   |  |
| 499           | 15                  |  |
| 500           | 19                  |  |
| 501           | 11                  |  |
| 502           | 11q14               |  |
| 503           | 17                  |  |
| 504           | 17                  |  |
| 506           | 17                  |  |
| 507           | 19                  |  |
| 508           | 2q36                |  |
| 509           | 20q11.21-13.13      |  |
| 510           | 19                  |  |
|               |                     |  |
| 511           | Xp11.1-11.22 5      |  |
| 512           |                     |  |
| 513           | 6                   |  |
| 514           | 6p24.1-25.3         |  |
| 515           | 12q                 |  |
| 516           | 22                  |  |
| 518           | 17                  |  |
| 519           | 18                  |  |
| 521           | 10q21               |  |
| 523           | 5                   |  |
| 524           | 8                   |  |
| 00002205Fg041 |                     |  |
| 525           | 8                   |  |
| 526           | 2q31                |  |
| 527           | 17                  |  |
| 528           | 16                  |  |
| 529           | 4q22-q24            |  |
| 530           | 22q12.3             |  |
| 531           | 18                  |  |
| 532           | 18                  |  |
| 534           | 10                  |  |
| 536           | 6                   |  |
| 539           | 1p33-34.3           |  |
| 540           | 10                  |  |
| 541           | 2                   |  |
| 542           | 10                  |  |
|               | 5                   |  |
| 543           |                     |  |
| 544           | 4                   |  |
| 545           | 12                  |  |
| 546           | 17                  |  |
| 547           | 16                  |  |
| 548           | 18                  |  |
| 551           | 16                  |  |
| 552           | 16                  |  |
| 553           | 17                  |  |
| 554           | Xq13.2-21.1         |  |
| 558           | 8                   |  |
| 559           | Xq13.3-21.2         |  |
| 560           | 11                  |  |
| 561           | 16q24.3             |  |
| L = - =       |                     |  |

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Table 7

| Table 7 |                     |  |
|---------|---------------------|--|
| SEQ ID  | Chromsomal location |  |
| 562     | 17                  |  |
| 563     | 11                  |  |
| 564     | 11                  |  |
| 565     | 10                  |  |
| 566     | X                   |  |
| 567     | 13q32.21-33.3       |  |
| 568     | 11                  |  |
| 569     | 20q11.21-q11.23     |  |
| 571     | X                   |  |
| 572     | 2p13                |  |
| 573     | 20                  |  |
| 574     | 10                  |  |
| 576     | 6q25.2-26           |  |
| 579     | 20                  |  |
| 580     | 17                  |  |
| 581     | 14q24.3             |  |
| 582     | X                   |  |
| 583     | 6p21-p12            |  |
| 584     | 11q22               |  |
| 588     | 16                  |  |
| 589     | 2                   |  |
| 590     | 16p13.3             |  |
| 591     | 17                  |  |
| 592     | 5                   |  |
|         | 5                   |  |
| 593     | 21q22.2             |  |
| 394     | 1p13.1-13.3         |  |
| 596     | 17                  |  |
| 597     | Xp11.4-21.2         |  |
| 598     | 1p34.1-36.11        |  |
| 599     | 12                  |  |
| 601     | 11                  |  |
| 602     | 11<br>14q21.1-q21.3 |  |
| 603     |                     |  |
| 604     | 11cen-q12.3         |  |
| 605     | 3                   |  |
| 606     | 11                  |  |
| 608     | 17                  |  |
| 609     | 13q22.1-31.1        |  |
| 610     | 5                   |  |
| 611     | 17                  |  |
| 613     | 13                  |  |
| 614     | 3                   |  |
| 616     | 11                  |  |
| 617     | 5                   |  |
| 620     | 1q23-25.            |  |
| 621     | 1q23-25.            |  |
| 622     | 17                  |  |
| 623     | 15                  |  |
| 624     | 15                  |  |
| 625     | 11                  |  |
| 626     | 14                  |  |
| 627     | 17                  |  |
| 628     | 12                  |  |
| 632     | 6p12.1-21.1         |  |
| 633     | 19q13.4             |  |

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Table 7

| Table 7 |                     |  |
|---------|---------------------|--|
| SEQ ID  | Chromsomal location |  |
| 634     | 4                   |  |
| 635     | 5                   |  |
| 637     | 9p13.1-13.3         |  |
| 638     | 17p11.2             |  |
| 639     | Xq22.1-22.3         |  |
| 640     | 20q13.3             |  |
| 641     | 1p22.3-31.2         |  |
| 642     | 1p22.3-31.2         |  |
| 643     | 10                  |  |
|         | 9q21.2-22.1         |  |
| 644     | 1                   |  |
| 645     |                     |  |
| 646     | 10q23-q24           |  |
| 648     | 8                   |  |
| 649     | 8                   |  |
| 650     | 16                  |  |
| 651     | 17pter-p13.1        |  |
| 652     | 19                  |  |
| 653     | X                   |  |
| 654     | 17                  |  |
| 655     | 9                   |  |
| 656     | 1                   |  |
| 657     | 18                  |  |
| 658     | 22                  |  |
| 659     | 11                  |  |
| 661     | 15                  |  |
| 663     | 12                  |  |
| 664     | 5                   |  |
| 665     | 19                  |  |
| 666     | Xq13.1-21.1.        |  |
| 667     | 10                  |  |
| 668     | 4                   |  |
| 669     | 17q21.33            |  |
|         | 17421.33            |  |
| 670     | 15q15               |  |
| 671     | 4q28                |  |
| 672     | 6                   |  |
| 673     | 15                  |  |
| 674     | 19                  |  |
| 675     | 2                   |  |
| 676     | 19                  |  |
| 679     | 6                   |  |
| 681     | 22                  |  |
| 682     | 11q14               |  |
| 683     | 15                  |  |
| 685     | Xp11.21-11.23       |  |
| 686     | 3                   |  |
| 687     | 19                  |  |
| 688     | 11                  |  |
| 689     | 20                  |  |
| 691     | 16q21               |  |
| 692     | 3                   |  |
| 693     | 9                   |  |
| 694     | 10                  |  |
| 695     | 2                   |  |
| 696     | 2                   |  |
| 697     | 17                  |  |
| U91     | 1/                  |  |

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Table 7

| Table 7     |                     |  |
|-------------|---------------------|--|
| SEQ ID      | Chromsomal location |  |
| 698         | 11p14               |  |
| 699         | 3q                  |  |
| 700         | 8p21-p12            |  |
| 701         | 19                  |  |
| 702         | 19                  |  |
| 703         | 22                  |  |
| 704         | 8p23-p22            |  |
| 705         | 19                  |  |
| 708         | 5                   |  |
| 710         | 17                  |  |
| 711         | 4                   |  |
| 712         | X                   |  |
| 713         | 1q41-q42            |  |
| 714         | 3                   |  |
| 715         | 1                   |  |
| 716         | 1                   |  |
| 717         | 18                  |  |
|             | 12                  |  |
| 718<br>721  | 6p21.3-22.2         |  |
| 722         | 13                  |  |
|             | 6                   |  |
| 724<br>725  | 13q14               |  |
|             | 20                  |  |
| 727         | 20q11.21-13.13      |  |
| 729         | 16                  |  |
| 730         | 16                  |  |
| 731         | 17                  |  |
| 732         |                     |  |
| 733         | 2                   |  |
| 734         | 15                  |  |
| 735         | 16                  |  |
| 737         | 15                  |  |
| 738         | 15                  |  |
| 739         | 15                  |  |
| 740         | 6q25.2-26           |  |
| 741         | 6925.2-26           |  |
| 742         | 6q25.2-26           |  |
| 743         | 4                   |  |
| 744         | 9q34                |  |
| 745         | 11q13               |  |
| 746         | 12                  |  |
| 749         | 20p11.1-11.22       |  |
| 751         | 9                   |  |
| 752         | 5q31-q32            |  |
| 753         | 2                   |  |
| 754         | 2                   |  |
| 755         | 19p11-q11           |  |
| 758         | 18                  |  |
| 760         | 16                  |  |
| 761         | 10q23.3             |  |
| 763         | 9                   |  |
| 764         | 13q22.1-31.1        |  |
| 765         | 14q23-q24           |  |
| 766         | 1                   |  |
| 767         | 1                   |  |
| 768         | 16                  |  |
| <del></del> |                     |  |

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Table 7

| SEQ ID     | Chromsomal location |
|------------|---------------------|
| 769        | 11                  |
| 770        | 9                   |
| 773        | 3                   |
| 775        | 13                  |
| 776        | 1                   |
| 777        | 12p13               |
| 779        | 17                  |
| 782        | 14                  |
| 784        | 17                  |
| 785        | 20q11.22-12         |
| 786        | 20q11.22-12         |
| 787        | 5                   |
| 788        | 8                   |
| 790        | 6q22.1-22.33        |
| 790        | 5                   |
| 791        | 13                  |
|            | 7                   |
| 793<br>794 |                     |
| 794        | 20p11.21-11.23      |
| 795        | 6q14.1-15           |
| 796        | 16                  |
| 797        | 9p13.1-13.3         |
| 798        | 2                   |
| 799        | 15q21.3             |
| 800        | 5q<br>8<br>8        |
| 801        | 8                   |
| 802        | 8                   |
| 803        | 3p                  |
| 805        | 10                  |
| 806        | 2                   |
| 807        | 17q21-q22           |
| 808        | 18q21               |
| 809        | 11                  |
| 811        | 2                   |
| 813        | 13                  |
| 814        | 11p13               |
| 815        | 12                  |
| 817        | 10                  |
| 818        | 2                   |
| 820        | 18                  |
| 822        | 3                   |
| 823        | 9                   |
| 824        | 3                   |
| 826        | 8q                  |
| 828        | 20                  |
| 829        | 11q23               |
| 830        | 19                  |
| 831        | 1                   |
| 836        | 17                  |
| 838        | 1                   |
| 839        | 17                  |
| 840        | 22q13.1             |
| 841        | 5                   |
| 842        | 1                   |
|            | 3                   |
| 843        |                     |
| 844        | 19q12               |

1160

Table 7

| Table 7    |                     |  |
|------------|---------------------|--|
| SEQ ID     | Chromsomal location |  |
| 845        | 19                  |  |
| 846        | 10                  |  |
| 847        | 16                  |  |
| 848        | 9                   |  |
| 849        | 3                   |  |
| 850        | 10                  |  |
| 851        | 15q21.2             |  |
| 852        | 8                   |  |
| 854        | 15q21.3             |  |
| 855        | 4                   |  |
| 856        | 1                   |  |
| 857        | 5                   |  |
| 858        | 3                   |  |
| 860        | 19q13.2             |  |
| 861        | 20q11.2-12          |  |
| 862        | 8                   |  |
| 863        | X                   |  |
| 864        | 3                   |  |
| 865        | 3                   |  |
| 866        | 10                  |  |
| 867        | 9                   |  |
| 868        | 11                  |  |
| 869        | 11                  |  |
| 870        | 11                  |  |
| 871        | 11                  |  |
| 872        | 7                   |  |
| 874        | 17                  |  |
| 875        | 2                   |  |
| 876        | 10                  |  |
| 878        | 2q14-q21            |  |
| 879        | 12                  |  |
| 880        | 19                  |  |
| 881        | 8q13                |  |
| 882        | 8                   |  |
| 883        | 17p13.3             |  |
| 884        | 12q                 |  |
| 885        | 3                   |  |
| 886        | 18                  |  |
| 887        | 12                  |  |
| 888        | 3p21.1-q13.13       |  |
| 889        | 19                  |  |
| 891        | Xp11.23-11.4        |  |
| 892        | 4                   |  |
| 893        | 1                   |  |
| 894        | X<br>Xq22.2-23      |  |
| 895        |                     |  |
| 896<br>897 | 19                  |  |
|            | 4                   |  |
| 898        |                     |  |
| 899        | 19                  |  |
| 900        | 19                  |  |
| 901        |                     |  |
| 902        | 19                  |  |
| 903        |                     |  |
| 904        | 18                  |  |

1161

Table 7

| SEQ ID Chromsomal location |                              |  |
|----------------------------|------------------------------|--|
| 908                        | 12q                          |  |
|                            | 19                           |  |
| 909                        | 9                            |  |
| 910                        | 8                            |  |
| 911                        |                              |  |
| 912                        | 12q23-q24<br>6               |  |
| 913                        |                              |  |
| 914                        | 19                           |  |
| 915                        | 1p36.11-36.33                |  |
| 916                        | 17                           |  |
| 917                        | 19                           |  |
| 918                        | 11q                          |  |
| 919                        | 19                           |  |
| 99990980Ff202              |                              |  |
| 920                        | 19                           |  |
| 99990980Ff202              |                              |  |
| 921                        | 3q<br>5                      |  |
| 924                        | 5                            |  |
| 925                        | 5                            |  |
| 926                        | 5                            |  |
| 927                        | 19                           |  |
| 928                        | 12q13                        |  |
| 932                        | 20                           |  |
| 933                        | 2p12-q11                     |  |
| 934                        | 2p12-q11                     |  |
| 935                        | 2p12-q11                     |  |
| 937                        | 7                            |  |
| 939                        | 16                           |  |
| 940                        | 6p11.2-q12.                  |  |
| 941                        | 3                            |  |
| 943                        | 10                           |  |
| 944                        | 22q11.2                      |  |
| 945                        | 22q11.2                      |  |
| 946                        | 9q31.3-33.3                  |  |
| 949                        | 2p13                         |  |
| 950                        | 17                           |  |
| 952                        | 1                            |  |
| 954                        | 22q12.3-13.2                 |  |
| 955                        | 16                           |  |
|                            | 17                           |  |
| 956<br>957                 | 17                           |  |
|                            | 19                           |  |
| 958                        | 19                           |  |
| 959                        | 4                            |  |
| 960                        |                              |  |
| 962                        | 17p11.2                      |  |
| 963                        | Xq21.31-22.1                 |  |
| 964                        | 16<br>19                     |  |
| 966                        | 1 19                         |  |
|                            |                              |  |
| 967                        | 1p34.1-36.11                 |  |
| 968                        | 1p34.1-36.11<br>1p34.1-36.11 |  |
|                            | 1p34.1-36.11                 |  |

1162 Table 8

| SEQ ID NO of Full-length | SEQ ID NO of Full-length | SEQ ID NO in Priority       |
|--------------------------|--------------------------|-----------------------------|
| Nucleotide Sequence      | Peptide Sequence         | Application USSN 60/324,631 |
|                          |                          |                             |
| 1                        | 972                      | 1                           |
| 2                        | 973                      | 2                           |
| 3                        | 974                      | 3                           |
| 4                        | 975                      | 4                           |
| 5                        | 976                      | 5                           |
| 6                        | 977                      | 6                           |
| 7                        | 978                      | 7                           |
| 8                        | 979                      | 9                           |
| 9                        | 980                      | 10                          |
| 10                       | 981                      | 11                          |
| 11                       | 982                      | 12                          |
| 12                       | 983                      | 13                          |
| 13                       | 984                      | 15                          |
| 14                       | 985                      | 16                          |
| 15                       | 986                      | 17                          |
| 16                       | 987                      | 18                          |
| 17                       | 988                      | 19                          |
| 18                       | 989                      | 20                          |
| 19                       | 990                      | 21                          |
| 20                       | 991                      | 22                          |
| 21                       | 992                      | 23                          |
| 22                       | 994                      | 24                          |
| 23                       | 995                      | 25                          |
| 24                       | 996                      | 26                          |
| 25                       | 997                      | 27                          |
| 26<br>27                 | 998                      | 28                          |
| 28                       | 999                      | 29                          |
| 29                       | 1000                     | 30                          |
| 30                       | 1000                     | 31                          |
| 31                       | 1002                     | 32                          |
| 32                       | 1003                     | 33                          |
| 33                       | 1004                     | 34                          |
| 34                       | 1005                     | 35                          |
| 35                       | 1006                     | 36                          |
| 36                       | 1007                     | 37                          |
| 37                       | 1008                     | 38                          |
| 38                       | 1009                     | 39                          |
| 39                       | 1010                     | 40                          |
| 40                       | 1011                     | 41                          |
| 41                       | 1012                     | 42 .                        |
| 42                       | 1013                     | 43                          |
| 43                       | 1014                     | 44                          |
| 44                       | 1015                     | 45                          |
| 45                       | 1016                     | 46                          |
| 46                       | 1017                     | 47                          |
| 47                       | 1018                     | 48                          |
| 48                       | 1019                     | 49                          |
| 49                       | 1020                     | 50                          |
| 50                       | 1021                     | 51                          |
| 51                       | 1022                     | 52                          |
| 52                       | 1023                     | 53                          |

1163 Table 8

| SEQ ID NO of Full-length | SEQ ID NO of Full-length | SEQ ID NO in Priority       |
|--------------------------|--------------------------|-----------------------------|
| Nucleotide Sequence      | Peptide Sequence         | Application USSN 60/324,631 |
| 53                       | 1024                     | 54                          |
| 54                       | 1025                     | 55                          |
| 55                       | 1026                     | 56                          |
| 56                       | 1027                     | 57                          |
| 57                       | 1028                     | 58                          |
| 58                       | 1029                     | 59                          |
| 59                       | 1030                     | 60                          |
| 60                       | 1031                     | 61                          |
| 61                       | 1032                     | 62                          |
| 62                       | 1033                     | 63                          |
| 63                       | 1034                     | 64                          |
| 64                       | 1035                     | 65                          |
| 65                       | 1036                     | 66                          |
| 66                       | 1037                     | 67                          |
| 67                       | 1038                     | 68                          |
| 68                       | 1039                     | 69                          |
| 69                       | 1040                     | 70                          |
| 70                       | 1041                     | 71                          |
| 71                       | 1042                     | 72                          |
| 72                       | 1043                     | 73                          |
| 73                       | 1044                     | 74                          |
| 74                       | 1045                     | 75                          |
| 75                       | 1046                     | 76                          |
| 76                       | 1047                     | 77                          |
| 77                       | 1048                     | 78                          |
| 78                       | 1049                     | 79                          |
| 79                       | 1050                     | 80                          |
| 80                       | 1051                     | 81                          |
| 81                       | 1052                     | 82                          |
| 82                       | 1053                     | 83                          |
| 83                       | 1054                     | 84                          |
| 84                       | 1055                     | 85                          |
| 85                       | 1056                     | 86                          |
| 86                       | 1057                     | 87                          |
| 87                       | 1058                     | 89                          |
| 88                       | 1059                     | 90                          |
| 89                       | 1060                     | 91                          |
| 90                       | 1061                     | 92                          |
| 91                       | 1062                     | 93                          |
| 92                       | 1063                     | 94                          |
| 93                       | 1064                     | 95                          |
| 94                       | 1065                     | 96                          |
| 95                       | 1066                     | 97                          |
| 96                       | 1067                     | 98                          |
| 97                       | 1068                     | 99                          |
| 98                       | 1069                     | 100                         |
| 99                       | 1070                     | 101                         |
| 100                      | 1071                     | 102                         |
| 101                      | 1072                     | 103                         |
| 102                      | 1073                     | 104                         |
| 103                      | 1074                     | 105                         |
| 104                      | 1075                     | 106                         |
| 105                      | 1076                     | 107                         |

1164 Table 8

| SEQ ID NO of Full-length | SEQ ID NO of Full-length | SEQ ID NO in Priority Application USSN |
|--------------------------|--------------------------|----------------------------------------|
| Nucleotide Sequence      | Peptide Sequence         | 60/324,631                             |
| 106                      | 1077                     | 108                                    |
| 107                      | 1078                     | 109                                    |
| 108                      | 1079                     | 110                                    |
| 109                      | 1080                     | 111                                    |
| 110                      | 1081                     | 112                                    |
| 111                      | 1082                     | 113                                    |
| 112                      | 1083                     | 114                                    |
| 113                      | 1084                     | 115                                    |
| 114                      | 1085                     | 116                                    |
| 115                      | 1086                     | 117                                    |
| 116                      | 1087                     | 118                                    |
| 117                      | 1088                     | 119                                    |
| 118                      | 1089                     | 120                                    |
| 119                      | 1090                     | 121                                    |
| 120                      | 1091                     | 122                                    |
| 121                      | 1092                     | 123                                    |
| 122                      | 1093                     | 124                                    |
| 123                      | 1094                     | 125                                    |
| 124                      | 1095                     | 126                                    |
| 125                      | 1096                     | 127                                    |
| 126                      | 1097                     | 128                                    |
| 127                      | 1098                     | 129                                    |
| 128                      | 1099                     | 130                                    |
| 129                      | 1100                     | 131                                    |
| 130                      | 1101                     | 132                                    |
| 131                      | 1102                     | 134                                    |
| 132                      | 1103                     | 135                                    |
| 133                      | 1104<br>1105             | 136                                    |
| 134                      | 1106                     | 137                                    |
| 135                      | 1107                     | 138                                    |
| 136                      | 1107                     | 139                                    |
| 137                      | 1108                     | 140                                    |
| 138                      | 1110                     | 141                                    |
| 139                      | 1111                     | 142                                    |
| 140                      | 1112                     | 143                                    |
| 141                      | 1113                     | 144                                    |
| 142                      | 1114                     | 145                                    |
| 143                      | 1114                     | 146                                    |
| 144                      | 1116                     | 147                                    |
| 145                      | 1117                     | 148                                    |
| 146<br>147               | 1117                     | 149                                    |
|                          | 1119                     | 150                                    |
| 148                      | 1120                     | 151                                    |
| 149                      | 1120                     | 152                                    |
| 150                      | 1122                     | 153                                    |
| 151                      | 1122                     | 154                                    |
| 152                      | 1123                     | 155                                    |
| 153                      | 1125                     | 156                                    |
| 154<br>155               | 1125                     | 157                                    |
| 156                      | 1127                     | 158                                    |
| 157                      | 1128                     | 159                                    |
| 158                      | 1129                     | 160                                    |

1165 Table 8

| SEQ ID NO of Full-length | SEQ ID NO of Full-length | SEQ ID NO in Priority |
|--------------------------|--------------------------|-----------------------|
| Nucleotide Sequence      | Peptide Sequence         | Application USSN      |
|                          |                          | 60/324,631            |
| 159                      | 1130                     | 161                   |
| 160                      | 1131                     | 162                   |
| 161                      | 1132                     | 163                   |
| 162                      | 1133                     | 164                   |
| 163                      | 1134                     | 165                   |
| 164                      | 1135                     | 166                   |
| 165                      | 1136                     | 167                   |
| 166                      | 1137                     | 168                   |
| 167                      | 1138                     | 169                   |
| 168                      | 1139                     | 170                   |
| 169                      | 1140                     | 171                   |
| 170                      | 1141                     | 172                   |
| 171                      | 1142                     | 173                   |
| 172                      | 1143                     | 174                   |
| 173                      | 1144                     | 175                   |
| 174                      | 1145                     | 176                   |
| 175                      | 1146                     | 177                   |
| 176                      | 1147                     | 178                   |
| 177                      | 1148                     | 179                   |
| 178                      | 1149                     | 180                   |
| 179                      | 1150                     | 181                   |
| 180                      | 1151                     | 182                   |
| 181                      | 1152                     | 183                   |
| 182                      | 1153                     | 184                   |
| 183                      | 1154                     | 185                   |
| 184                      | 1155                     | 186                   |
| 185                      | 1156                     | 187                   |
| 186                      | 1157                     | 188                   |
| 187                      | 1158                     | 189                   |
| 188                      | 1159                     | 190                   |
| 189                      | 1160                     | 191                   |
| 190                      | 1161                     | 192                   |
| 191                      | 1162                     | 193                   |
| 192                      | 1163                     | 194                   |
| 193                      | 1164                     | 195                   |
| 194                      | 1165                     | 196                   |
| 195                      | 1166                     | 197                   |
| 196                      | 1167                     | 198                   |
| 197                      | 1168                     | 199                   |
| 198                      | 1169                     | 200                   |
| 199                      | 1170                     | 201                   |
| 200                      | 1171                     | 202                   |
| 201                      | 1172                     | 203                   |
| 202                      | 1173                     | 204                   |
| 203                      | 1174                     | 205                   |
| 204                      | 1175                     | 206                   |
| 205                      | 1176                     | 207                   |
| 206                      | 1177                     | 208                   |
| 207                      | 1178                     | 209                   |
| 208                      | 1179                     | 210                   |
| 209                      | 1180                     | 211                   |
| 210                      | 1181                     | 212                   |
| 211                      | 1182                     | 213                   |

1166 Table 8

| SEQ ID NO of Full-length<br>Nucleotide Sequence | SEQ ID NO of Full-length Peptide Sequence | SEQ ID NO in Priority Application USSN |
|-------------------------------------------------|-------------------------------------------|----------------------------------------|
| Nucleotide Sequence                             | replide Sequence                          | 60/324,631                             |
| 212                                             | 1183                                      | 214                                    |
| 213                                             | 1184                                      | 215                                    |
| 214                                             | 1185                                      | 216                                    |
| 215                                             | 1186                                      | 217                                    |
| 216                                             | 1187                                      | 218                                    |
| 217                                             | 1188                                      | 219                                    |
| 218                                             | 1189                                      | 220                                    |
| 219                                             | 1190                                      | 221                                    |
| 220                                             | 1191                                      | 222                                    |
| 221                                             | 1192                                      | 223                                    |
| 222                                             | 1193                                      | 224                                    |
| 223                                             | 1194                                      | 225                                    |
| 224                                             | 1195                                      | 226                                    |
| 225                                             | 1196                                      | 227                                    |
| 226                                             | 1197                                      | 228                                    |
| 227                                             | 1198                                      | 229                                    |
| 228                                             | 1199                                      | 230                                    |
| 229                                             | 1200                                      | 231                                    |
| 230                                             | 1201                                      | 232                                    |
| 231                                             | 1202                                      | 233                                    |
| 232                                             | 1203                                      | 234                                    |
| 233                                             | 1204                                      | 235                                    |
| 234                                             | 1205                                      | 236                                    |
| 235                                             | 1206                                      | 237                                    |
| 236                                             | 1207                                      | 238                                    |
| 237                                             | 1208                                      | 239                                    |
| 238                                             | 1208                                      | 240                                    |
| 239                                             | 1210                                      | 241                                    |
| 240                                             | 1210                                      | 242                                    |
| 241                                             | 1211                                      | 243                                    |
|                                                 | 1212                                      | 244                                    |
| 242                                             |                                           | 245                                    |
| 243                                             | 1214                                      | 246                                    |
| 244                                             | 1215                                      | 247                                    |
| 245                                             | 1216                                      |                                        |
| 246                                             | 1217                                      | 248                                    |
| 247                                             | 1218                                      | 249                                    |
| 248                                             | 1219                                      | 250                                    |
| 249                                             | 1220                                      | 251                                    |
| 250                                             | 1221                                      | 252                                    |
| 251                                             | 1222                                      | 253                                    |
| 252                                             | 1223                                      | 254                                    |
| 253                                             | 1224                                      | 255                                    |
| 254                                             | 1225                                      | 256                                    |
| 255                                             | 1226                                      | 257                                    |
| 256                                             | 1227                                      | 258                                    |
| 257                                             | 1228                                      | 259                                    |
| 258                                             | 1229                                      | 260                                    |
| 259                                             | 1230                                      | 261                                    |
| 260                                             | 1231                                      | 262                                    |
| 261                                             | 1232                                      | 263                                    |
| 262                                             | 1233                                      | 264                                    |
| 263                                             | 1234                                      | 265                                    |
| 264                                             | 1235                                      | 266                                    |

1167 Table 8

| SEQ ID NO of Full-length | SEQ ID NO of Full-length | SEQ ID NO in Priority       |
|--------------------------|--------------------------|-----------------------------|
| Nucleotide Sequence      | Peptide Sequence         | Application USSN 60/324,631 |
| 265                      | 1236                     | 267                         |
| 266                      | 1237                     | 268                         |
| 267                      | 1238                     | 269                         |
| 268                      | 1239                     | 270                         |
| 269                      | 1240                     | 271                         |
| 270                      | 1241                     | 272                         |
| 271                      | 1242                     | 273                         |
| 272                      | 1243                     | 274                         |
| 273                      | 1244                     | 275                         |
| 274                      | 1245                     | 276                         |
| 275                      | 1246                     | 277                         |
| 276                      | 1247                     | 278                         |
| 277                      | 1248                     | 279                         |
| 278                      | 1249                     | 280                         |
| 279                      | 1250                     | 281                         |
| 280                      | 1251                     | 282                         |
| 281                      | 1252                     | 283                         |
| 282                      | 1252                     | 284                         |
|                          | 1254                     | 285                         |
| 283                      | 1255                     | 286                         |
| 284                      | 1256                     | 287                         |
| 285                      | 1257                     | 288                         |
| 286                      |                          | 289                         |
| 287                      | 1258                     | 290                         |
| 288                      | 1259                     | 291                         |
| 289                      | 1260                     | 292                         |
| 290                      | 1261                     | 293                         |
| 291                      | 1262                     |                             |
| 292                      | 1263                     | 294                         |
| 293                      | 1264                     | 295                         |
| 294                      | 1265                     | 296                         |
| 295                      | 1266                     | 297                         |
| 296                      | 1267                     | 298                         |
| 297                      | 1268                     | 299                         |
| 298                      | 1269                     | 300                         |
| 299                      | 1270                     | 301                         |
| 300                      | 1271                     | 302                         |
| 301                      | 1272                     | 303                         |
| 302                      | 1273                     | 304                         |
| 303                      | 1274                     | 305                         |
| 304                      | 1275                     | 306                         |
| 305                      | 1276                     | 307                         |
| 306                      | 1277                     | 308                         |
| 307                      | 1278                     | 309                         |
| 308                      | 1279                     | 310                         |
| 309                      | 1280                     | 311                         |
| 310                      | 1281                     | 312                         |
| 311                      | 1282                     | 313                         |
| 312                      | 1283                     | 314                         |
| 313                      | 1284                     | 315                         |
| 314                      | 1285                     | 316                         |
| 315                      | 1286                     | 317                         |
| 316                      | 1287                     | 318                         |
| 317                      | 1288                     | 319                         |

1168 Table 8

| SEQ ID NO of Full-length | SEQ ID NO of Full-length<br>Peptide Sequence | SEQ ID NO in Priority Application USSN |
|--------------------------|----------------------------------------------|----------------------------------------|
| Nucleotide Sequence      | Peptide Sequence                             | 60/324,631                             |
| 210                      | 1289                                         | 320                                    |
| 318                      | 1290                                         | 321                                    |
| 319                      | 1290                                         | 322                                    |
| 320                      | 1291                                         | 323                                    |
| 321                      | 1292                                         | 324                                    |
| 322                      | 1293                                         | 325                                    |
| 323                      | 1294                                         | 326                                    |
| 324                      | 1295                                         | 327                                    |
| 325                      | 1297                                         | 328                                    |
| 326                      | 1297                                         | 329                                    |
| 327                      | 1298                                         | 330                                    |
| 328                      |                                              | 331                                    |
| 329                      | 1300                                         | 332                                    |
| 330                      | 1301                                         |                                        |
| 331                      | 1302                                         | 333                                    |
| 332                      | 1303                                         | 335                                    |
| 333                      | 1304                                         |                                        |
| 334                      | 1305                                         | 336                                    |
| 335                      | 1306                                         | 337                                    |
| 336                      | 1307                                         | 338                                    |
| 337                      | 1308                                         | 339                                    |
| 338                      | 1309                                         | 340                                    |
| 339                      | 1310                                         | 341                                    |
| 340                      | 1311                                         | 342                                    |
| 341                      | 1312                                         | 343                                    |
| 342                      | 1313                                         | 344                                    |
| 343                      | 1314                                         | 345                                    |
| 344                      | 1315                                         | 346                                    |
| 345                      | 1316                                         | 347                                    |
| 346                      | 1317                                         | 348                                    |
| 347                      | 1318                                         | 349                                    |
| 348                      | 1319                                         | 350                                    |
| 349                      | 1320                                         | 351                                    |
| 350                      | 1321                                         | 352                                    |
| 351                      | 1322                                         | 353                                    |
| 352                      | 1323                                         | 354                                    |
| 353                      | 1324                                         | 355                                    |
| 354                      | 1325                                         | 356                                    |
| 355                      | 1326                                         | 357                                    |
| 356                      | 1327                                         | 358                                    |
| 357                      | 1328                                         | 359                                    |
| 358                      | 1329                                         | 360                                    |
| 359                      | 1330                                         | 361                                    |
| 360                      | 1331                                         | 362                                    |
| 361                      | 1332                                         | 363                                    |
| 362                      | 1333                                         | 364                                    |
| 363                      | 1334                                         | 365                                    |
|                          | 1335                                         | 366                                    |
| 364                      | 1336                                         | 367                                    |
| 365                      |                                              | 368                                    |
| 366                      | 1337                                         | 369                                    |
| 367                      | 1338                                         |                                        |
| 368                      | 1339                                         | 370                                    |
| 369                      |                                              |                                        |

1169 Table 8

| SEQ ID NO of Full-length   SEQ ID NO of Full-length   SEQ ID NO in Prior |                                       |                                |
|--------------------------------------------------------------------------|---------------------------------------|--------------------------------|
| Nucleotide Sequence                                                      | Peptide Sequence                      | Application USSN<br>60/324,631 |
| 371                                                                      | 1342                                  | 373                            |
| 372                                                                      | 1343                                  | 374                            |
| 373                                                                      | 1344                                  | 375                            |
| 374                                                                      | 1345                                  | 376                            |
| 375                                                                      | 1346                                  | 377                            |
| 376                                                                      | 1347                                  | 378                            |
| 377                                                                      | 1348                                  | 379                            |
|                                                                          | 1349                                  | 380                            |
| 378                                                                      | 1350                                  | 381                            |
| 379                                                                      | 1351                                  | 382                            |
| 380                                                                      | 1352                                  | 383                            |
| 381                                                                      |                                       | 384                            |
| 382                                                                      | 1353                                  | 385                            |
| 383                                                                      | 1354                                  |                                |
| 384                                                                      | 1355                                  | 386                            |
| 385                                                                      | 1356                                  | 387                            |
| 386                                                                      | 1357                                  | 388                            |
| 387                                                                      | 1358                                  | 389                            |
| 388                                                                      | 1359                                  | 390                            |
| 389                                                                      | 1360                                  | 391                            |
| 390                                                                      | 1361                                  | 392                            |
| 391                                                                      | 1362                                  | 393                            |
| 392                                                                      | 1363                                  | 394                            |
| 393                                                                      | 1364                                  | 395                            |
| 394                                                                      | 1365                                  | 396                            |
| 395                                                                      | 1366                                  | 397                            |
| 396                                                                      | 1367                                  | 398                            |
| 397                                                                      | 1368                                  | 399                            |
| 398                                                                      | 1369                                  | 400                            |
| 399                                                                      | 1370                                  | 401                            |
| 400                                                                      | 1371                                  | 402                            |
| 401                                                                      | 1372                                  | 403                            |
| 402                                                                      | 1373                                  | 404                            |
| 403                                                                      | 1374                                  | 405                            |
| 404                                                                      | 1375                                  | 406                            |
| 405                                                                      | 1376                                  | 407                            |
| 406                                                                      | 1377                                  | 408                            |
| 407                                                                      | 1378                                  | 409                            |
| 408                                                                      | 1379                                  | 410                            |
|                                                                          | 1380                                  | 411                            |
| 409                                                                      | 1381                                  | 412                            |
| 410                                                                      | 1382                                  | 413                            |
| 411                                                                      | 1382                                  | 414                            |
| 412                                                                      | · · · · · · · · · · · · · · · · · · · | 415                            |
| 413                                                                      | 1384                                  |                                |
| 414                                                                      | 1385                                  | 416                            |
| 415                                                                      | 1386                                  | 417                            |
| 416                                                                      | 1387                                  | 418                            |
| 417                                                                      | 1388                                  | 419                            |
| 418                                                                      | 1389                                  | 420                            |
| 419                                                                      | 1390                                  | 421                            |
| 420                                                                      | 1391                                  | 422                            |
| 421                                                                      | 1392                                  | 423                            |
| 422                                                                      | 1393                                  | 424                            |
| 423                                                                      | 1394                                  | 425                            |

1170 Table 8

| SEQ ID NO of Full-length<br>Nucleotide Sequence | SEQ ID NO of Full-length<br>Peptide Sequence | SEQ ID NO in Priority Application USSN |
|-------------------------------------------------|----------------------------------------------|----------------------------------------|
|                                                 |                                              | 60/324,631                             |
| 424                                             | 1395                                         | 426                                    |
| 425                                             | 1396                                         | 427                                    |
| 426                                             | 1397                                         | 428                                    |
| 427                                             | 1398                                         | 429                                    |
| 428                                             | 1399                                         | 430                                    |
| 429                                             | 1400                                         | 431                                    |
| 430                                             | 1401                                         | 432                                    |
| 431                                             | 1402                                         | 433                                    |
| 432                                             | 1403                                         | 434                                    |
| 433                                             | 1404                                         | 435                                    |
| 434                                             | 1405                                         | 436                                    |
| 435                                             | 1406                                         | 437                                    |
| 436                                             | 1407                                         | 438                                    |
| 437                                             | 1408                                         | 439                                    |
| 438                                             | 1409                                         | 440                                    |
| 439                                             | 1410                                         | 441                                    |
| 440                                             | 1411                                         | 442                                    |
| 441                                             | 1412                                         | 443                                    |
| 442                                             | 1413                                         | 444                                    |
| 443                                             | 1414                                         | 445                                    |
| 444                                             | 1415                                         | 446                                    |
| 445                                             | 1416                                         | 447                                    |
| 446                                             | 1417                                         | 448                                    |
| 447                                             | 1418                                         | 449                                    |
| 448                                             | 1419                                         | 450                                    |
| 449                                             | 1420                                         | 451                                    |
| 450                                             | 1421                                         | 452                                    |
| 451                                             | 1422                                         | 453                                    |
| 452                                             | 1423                                         | 454                                    |
| 453                                             | 1424                                         | 455                                    |
| 454                                             | 1425                                         | 456                                    |
| 455                                             | 1426                                         | 457                                    |
| 456                                             | 1427                                         | 458                                    |
| 457                                             | 1428                                         | 459                                    |
|                                                 |                                              |                                        |
| 458                                             | 1429                                         | 460                                    |
| 459                                             | 1430                                         | 461                                    |
| 460                                             | 1431                                         | 462                                    |
| 461                                             | 1432                                         | 463                                    |
| 462                                             | 1433                                         | 464                                    |
| 463                                             | 1434                                         | 465                                    |
| 464                                             | 1435                                         | 466                                    |
| 465                                             | 1436                                         | 467                                    |
| 466                                             | 1437                                         | 468                                    |
| 467                                             | 1438                                         | 469                                    |
| 468                                             | 1439                                         | 470                                    |
| 469                                             | 1440                                         | 471                                    |
| 470                                             | 1441                                         | 472                                    |
| 471                                             | 1442                                         | 473                                    |
| 472                                             | 1443                                         | 474                                    |
| 473                                             | 1444                                         | 475                                    |
| 474                                             | 1445                                         | 476                                    |
| 475                                             | 1446                                         | 477                                    |
| 476                                             | 1447                                         | 478                                    |
|                                                 |                                              |                                        |

1171 Table 8

| SEQ ID NO of Full-length<br>Nucleotide Sequence | SEQ ID NO of Full-length<br>Peptide Sequence | SEQ ID NO in Priority Application USSN 60/324,631 |
|-------------------------------------------------|----------------------------------------------|---------------------------------------------------|
| 477                                             | 1448                                         | 479                                               |
| 478                                             | 1449                                         | 480                                               |
| 479                                             | 1450                                         | 481                                               |
| 480                                             | 1451                                         | 482                                               |
| 481                                             | 1452                                         | 483                                               |
| 482                                             | 1453                                         | 484                                               |
| 483                                             | 1454                                         | 485                                               |
| 484                                             | 1455                                         | 486                                               |
| 485                                             | 1456                                         | 487                                               |
| 486                                             | 1457                                         | 488                                               |
| 487                                             | 1458                                         | 489                                               |
| 488                                             | 1459                                         | 490                                               |
| 489                                             | 1460                                         | 491                                               |
| 490                                             | 1461                                         | 492                                               |
| 491                                             | 1462                                         | 493                                               |
| 492                                             | 1463                                         | 494                                               |
| 493                                             | 1464                                         | 495                                               |
| 494                                             | 1465                                         | 496                                               |
| 495                                             | 1466                                         | 497                                               |
| 496                                             | 1467                                         | 498                                               |
| 497                                             | 1468                                         | 499                                               |
| 498                                             | 1469                                         | 500                                               |
| 499                                             | 1470                                         | 501                                               |
| 500                                             | 1471                                         | 502                                               |
| 501                                             | 1472                                         | 503                                               |
| 502                                             | 1473                                         | 504                                               |
| 503                                             | 1474                                         | 505                                               |
| 504                                             | 1475                                         | 506                                               |
| 505                                             | 1476                                         | 507                                               |
| 506                                             | 1477                                         | 508                                               |
| 507                                             | 1478                                         | 509                                               |
| 508                                             | 1479                                         | 510                                               |
| 509                                             | 1480                                         | 511                                               |
| 510                                             | 1481                                         | 512                                               |
| 511                                             | 1482                                         | 513                                               |
| 512                                             | 1483                                         | 514                                               |
| 513                                             | 1484                                         | 515                                               |
| 514                                             | 1485                                         | 516                                               |
| 515                                             | 1486                                         | 517                                               |
| 516                                             | 1487                                         | 518                                               |
| 517                                             | 1488                                         | 519                                               |
| 518                                             | 1489                                         | 520                                               |
| 519                                             | 1490                                         | 521                                               |
| 520                                             | 1491                                         | 522                                               |
| 521                                             | 1492                                         | 523                                               |
| 522                                             | 1493                                         | 524                                               |
| 523                                             | 1494                                         | 525                                               |
| 524                                             | 1495                                         | 526                                               |
| 525                                             | 1496                                         | 527                                               |
| 526                                             | 1497                                         | 528                                               |
| 527                                             | 1498                                         | 529                                               |
| 528                                             | 1499                                         | 530                                               |
| 529                                             | 1500                                         | 531                                               |

1172 Table 8

| CEO ID NO - CE-II I                             | Table 8                                      | CEC ID NO : Delete                                |
|-------------------------------------------------|----------------------------------------------|---------------------------------------------------|
| SEQ ID NO of Full-length<br>Nucleotide Sequence | SEQ ID NO of Full-length<br>Peptide Sequence | SEQ ID NO in Priority Application USSN 60/324,631 |
| 530                                             | 1501                                         | 532                                               |
| 531                                             | 1502                                         | 533                                               |
| 532                                             | 1503                                         | 534                                               |
| 533                                             | 1504                                         | 535                                               |
| 534                                             | 1505                                         | 536                                               |
| 535                                             | 1506                                         | 537                                               |
| 536                                             | 1507                                         | 538                                               |
| 537                                             | 1508                                         | 539                                               |
| 538                                             | 1509                                         | 540                                               |
| 539                                             | 1510                                         | 541                                               |
| 540                                             | 1510                                         |                                                   |
|                                                 |                                              | 542                                               |
| 541                                             | 1512                                         | 543                                               |
| 542                                             | 1513                                         | 544                                               |
| 543                                             | 1514                                         | 545                                               |
| 544                                             | 1515                                         | 546                                               |
| 545                                             | 1516                                         | 547                                               |
| 546                                             | 1517                                         | 548                                               |
| 547                                             | 1518                                         | 549                                               |
| 548                                             | 1519                                         | 550                                               |
| 549                                             | 1520                                         | 551                                               |
| 550                                             | 1521                                         | 552                                               |
| 551                                             | 1522                                         | 553                                               |
| 552                                             | 1523                                         | 554                                               |
| 553                                             | 1524                                         | 555                                               |
| 554                                             | 1525                                         | 556                                               |
| 555                                             | 1526                                         | 557                                               |
| 556                                             | 1527                                         | 558                                               |
| 557                                             | 1528                                         | 559                                               |
| 558                                             | 1529                                         | 560                                               |
| 559                                             | 1530                                         |                                                   |
| 560                                             |                                              | 561                                               |
|                                                 | 1531                                         | 562                                               |
| 561                                             | 1532                                         | 563                                               |
| 562                                             | 1533                                         | 564                                               |
| 563                                             | 1534                                         | 565                                               |
| 564                                             | 1535                                         | 566                                               |
| 565                                             | 1536                                         | 567                                               |
| 566                                             | 1537                                         | 568                                               |
| 567                                             | 1538                                         | 569                                               |
| 568                                             | 1539                                         | 570                                               |
| 569                                             | 1540                                         | 571                                               |
| 570                                             | 1541                                         | 572                                               |
| 571                                             | 1542                                         | 573                                               |
| 572                                             | 1543                                         | 574                                               |
| 573                                             | 1544                                         | 575                                               |
| 574                                             | 1545                                         | 576                                               |
| 575                                             | 1546                                         | 577                                               |
| 576                                             | 1547                                         | 578                                               |
|                                                 |                                              |                                                   |
| 577                                             | 1548                                         | 579                                               |
| 578                                             | 1549                                         | 580                                               |
| 579                                             | 1550                                         | 581                                               |
| 580                                             | 1551                                         | 582                                               |
| 581                                             | 1552                                         | 583                                               |
| 582                                             | 1553                                         | 584                                               |

1173 Table 8

| CEO ID NO CE UL A                               | Table o                                      | CEO TO NO ! D ! !!                                |
|-------------------------------------------------|----------------------------------------------|---------------------------------------------------|
| SEQ ID NO of Full-length<br>Nucleotide Sequence | SEQ ID NO of Full-length<br>Peptide Sequence | SEQ ID NO in Priority Application USSN 60/324,631 |
| 583                                             | 1554                                         | 585                                               |
| 584                                             | 1555                                         | 586                                               |
| 585                                             | 1556                                         | 587                                               |
| 586                                             | 1557                                         | 588                                               |
| 587                                             | 1558                                         | 589                                               |
| 588                                             | 1559                                         | 590                                               |
| 589                                             | 1560                                         | 591                                               |
| 590                                             | 1561                                         | 592                                               |
| 591                                             | 1562                                         | 593                                               |
| 592                                             | 1563                                         | 594                                               |
| 593                                             | 1564                                         | 595                                               |
| 594                                             | 1565                                         | 596                                               |
| 595                                             | 1566                                         | 597                                               |
| 596                                             | 1567                                         | 598                                               |
| 597                                             |                                              |                                                   |
| 598                                             | 1568                                         | 599                                               |
|                                                 | 1569                                         | 600                                               |
| 599                                             | 1570                                         | 601                                               |
| 600                                             | 1571                                         | 602                                               |
| 601                                             | 1572                                         | 603                                               |
| 602                                             | 1573                                         | 604                                               |
| 603                                             | 1574                                         | 605                                               |
| 604                                             | 1575                                         | 606                                               |
| 605                                             | 1576                                         | 607                                               |
| 606                                             | 1577                                         | 608                                               |
| 607                                             | 1578                                         | 609                                               |
| 608                                             | 1579                                         | 610                                               |
| 609                                             | 1580                                         | 611                                               |
| 610                                             | 1581                                         | 612                                               |
| 611                                             | 1582                                         | 613                                               |
| 612                                             | 1583                                         | 614                                               |
| 613                                             | 1584                                         | 615                                               |
| 614                                             | 1585                                         | 616                                               |
| 615                                             | 1586                                         | 617                                               |
| 616                                             | 1587                                         | 618                                               |
| 617                                             | 1588                                         | 619                                               |
| 618                                             | 1589                                         | 620                                               |
| 619                                             | 1590                                         | 621                                               |
| 620                                             | 1591                                         | 622                                               |
| 621                                             | 1592                                         | 623                                               |
| 622                                             | 1593                                         | 624                                               |
| 623                                             | 1594                                         | 625                                               |
| 624                                             | 1595                                         |                                                   |
| 625                                             |                                              | 626                                               |
|                                                 | 1596                                         | 627                                               |
| 626                                             | 1597                                         | 628                                               |
| 627                                             | 1598                                         | 629                                               |
| 628                                             | 1599                                         | 630                                               |
| 629                                             | 1600                                         | 631                                               |
| 630                                             | 1601                                         | 632                                               |
| 631                                             | 1602                                         | 633                                               |
| 632                                             | 1603                                         | 634                                               |
| 633                                             | 1604                                         | 635                                               |
| 634                                             | 1605                                         | 636                                               |
| 635                                             | 1606                                         | 637                                               |

1174 Table 8

| SEQ ID NO of Full-length | SEQ ID NO of Full-length | SEQ ID NO in Priority |
|--------------------------|--------------------------|-----------------------|
| Nucleotide Sequence      | Peptide Sequence         | Application USSN      |
|                          |                          | 60/324,631            |
| 636                      | 1607                     | 638                   |
| 637                      | 1608                     | 639                   |
| 638                      | 1609                     | 640                   |
| 639                      | 1610                     | 641                   |
| 640                      | 1611                     | 642                   |
| 641                      | 1612                     | 643                   |
| 642                      | 1613                     | 644                   |
| 643                      | 1614                     | 645                   |
| 644                      | 1615                     | 646                   |
| 645                      | 1616                     | 647                   |
| 646                      | 1617                     | 648                   |
| 647                      | 1618                     | 649                   |
| 648                      | 1619                     | 650                   |
| 649                      | 1620                     | 651                   |
| 650                      | 1621                     | 652                   |
| 651                      | 1622                     | 653                   |
| 652                      | 1623                     | 654                   |
| 653                      | 1624                     | 655                   |
| 654                      | 1625                     | 656                   |
| 655                      | 1626                     | 657                   |
| 656                      | 1627                     | 658                   |
| 657                      | 1628                     | 659                   |
| 658                      | 1629                     | 660                   |
| 659                      | 1630                     | 661                   |
| 660                      | 1631                     | 662                   |
| 661                      | 1632                     | 663                   |
| 662                      | 1633                     | 664                   |
| 663                      | 1634                     | 665                   |
| 664                      | 1635                     | 666                   |
| 665                      | 1636                     | 667                   |
| 666                      | 1637                     | 668                   |
| 667                      | 1638                     | 669                   |
| 668                      | 1639                     | 670                   |
| 669                      | 1640                     | 671                   |
| 670                      | 1641                     | 672                   |
| 671                      | 1642                     | 673                   |
| 672                      | 1643                     | 674                   |
| 673                      | 1644                     | 675                   |
| 674                      | 1645                     | 676                   |
| 675                      | 1646                     | 677                   |
| 676                      | 1647                     | 678                   |
| 677                      | 1648                     | 679                   |
| 678<br>679               | 1649                     | 680                   |
|                          | 1650                     | 681                   |
| 680                      | 1651                     | 682                   |
| 681                      | 1652                     | 683                   |
| 682                      | 1653                     | 684                   |
| 683                      | 1654                     | 685                   |
| 684                      | 1655                     | 686                   |
| 685                      | 1656                     | 687                   |
| 686                      | 1657                     | 688                   |
| 687                      | 1658                     | 689                   |
| 688                      | 1659                     | 690                   |

1175 Table 8

| SEQ ID NO of Full-length | SEQ ID NO of Full-length | SEQ ID NO in Priority          |
|--------------------------|--------------------------|--------------------------------|
| Nucleotide Sequence      | Peptide Sequence         | Application USSN<br>60/324,631 |
| 689                      | 1660                     | 691                            |
| 690                      | 1661                     | 692                            |
| 691                      | 1662                     | 693                            |
| 692                      | 1663                     | 694                            |
| 693                      | 1664                     | 695                            |
| 694                      | 1665                     | 696                            |
| 695                      | 1666                     | 697                            |
| 696                      | 1667                     | 698                            |
| 697                      | 1668                     | 699                            |
| 698                      | 1669                     | 700                            |
| 699                      | 1670                     | 701                            |
| 700                      | 1671                     | 702                            |
| 701                      | 1672                     | 703                            |
| 702                      | 1673                     | 704                            |
| 703                      | 1674                     | 705                            |
| 704                      | 1675                     | 706                            |
| 705                      | 1676                     | 707                            |
| 706                      | 1677                     | 708                            |
| 707                      | 1678                     | 709                            |
| 708                      | 1679                     | 710                            |
| 709                      | 1680                     | 711                            |
| 710                      | 1681                     | 712                            |
| 711                      | 1682                     | 713                            |
| 712                      | 1683                     | 714                            |
| 713                      | 1684                     | 715                            |
| 714                      | 1685                     | 716                            |
| 715                      | 1686                     | 717                            |
| 716                      | 1687                     | 718                            |
| 717                      | 1688                     | 719                            |
| 718                      | 1689                     | 720                            |
| 719                      | 1690                     | 721                            |
| 720                      | 1691                     | 722                            |
| 721                      | 1692                     | 723                            |
| 722                      | 1693                     | 724                            |
| 723                      | 1694                     | 725                            |
| 724                      | 1695                     | 726                            |
| 725                      | 1696                     | 727                            |
| 726                      | 1697                     | 728                            |
| 727                      | 1698                     | 729                            |
| 728                      | 1699                     | 730                            |
| 729                      | 1700                     | 731                            |
| 730                      | 1701                     | 732                            |
| 731                      | 1702                     | 733                            |
| 732                      | 1703                     | 734                            |
| 733                      | 1704                     | 735                            |
| 734                      | 1705                     | 736                            |
| 735                      | 1706                     | 737                            |
| 736                      | 1707                     | 738                            |
| 737                      | 1708                     | 739                            |
| 738                      | 1709                     | 740                            |
| 739                      | 1710                     | 741                            |
|                          |                          |                                |
| 740                      | 1711                     | 742                            |

1176 Table 8

| SEQ ID NO of Full-length | Table 8 SEQ ID NO of Full-length | SEQ ID NO in Priority       |
|--------------------------|----------------------------------|-----------------------------|
| Nucleotide Sequence      | Peptide Sequence                 | Application USSN 60/324,631 |
| 742                      | 1713                             | 744                         |
| 743                      | 1714                             | 745                         |
| 744                      | 1715                             | 746                         |
| 745                      | 1716                             | 747                         |
| 746                      | 1717                             | 748                         |
| 747                      | 1718                             | 749                         |
| 748                      | 1719                             | 750                         |
| 749                      | 1720                             | 751                         |
| 750                      | 1721                             | 752                         |
| 751                      | 1722                             | 753                         |
| 752                      | 1723                             | 754                         |
| 753                      | 1724                             | 755                         |
| 754                      | 1725                             | 756                         |
| 755                      | 1726                             | 757                         |
| 756                      | 1727                             | 758                         |
| 757                      | 1728                             | 759                         |
| 758                      | 1729                             | 760                         |
| 759                      | 1730                             | 761                         |
| 760                      | 1731                             | 762                         |
| 761                      | 1732                             | 763                         |
| 762                      | 1733                             | 764                         |
| 763                      | 1734                             | 765                         |
| 764                      | 1735                             | 766                         |
| 765                      | 1736                             | 767                         |
| 766                      | 1737                             | 768                         |
| 767                      | 1738                             | 769                         |
| 768                      | 1739                             | 770                         |
| 769                      | 1740                             | 771                         |
| 770                      | 1741                             | 772                         |
| 771                      | 1742                             | 773                         |
| 772                      | 1743                             | 774                         |
| 773                      | 1744                             | 775                         |
| 774                      | 1745                             | 776                         |
| 775                      | 1746                             | 777                         |
| 776                      | 1747                             | 778                         |
| 777                      | 1748                             | 779                         |
| 778                      | 1749                             | 780                         |
| 779                      | 1750                             | 781                         |
| 780                      | 1751                             | 782                         |
| 781                      | 1752                             | 783                         |
| 782                      | 1753                             | 784                         |
| 783<br>784               | 1754                             | 785                         |
| 785                      | 1755                             | 786                         |
|                          | 1756                             | 787                         |
| 786                      | 1757                             | 788                         |
| 787                      | 1758                             | 789                         |
| 788                      | 1759                             | 790                         |
| 789                      | 1760                             | 791                         |
| 790                      | 1761                             | 792                         |
| 791                      | 1762                             | 793                         |
| 792                      | 1763                             | 794                         |
| 793                      | 1764                             | 795                         |
| 794                      | 1765                             | 796                         |

1177 Table 8

| Table 8                                         |                                              |                                                         |  |  |
|-------------------------------------------------|----------------------------------------------|---------------------------------------------------------|--|--|
| SEQ ID NO of Full-length<br>Nucleotide Sequence | SEQ ID NO of Full-length<br>Peptide Sequence | SEQ ID NO in Priority<br>Application USSN<br>60/324,631 |  |  |
| 795                                             | 1766                                         | 797                                                     |  |  |
| 796                                             | 1767                                         | 798                                                     |  |  |
| 797                                             | 1768                                         | 799                                                     |  |  |
| 798                                             | 1769                                         | 800                                                     |  |  |
| 799                                             | 1770                                         | 801                                                     |  |  |
| 800                                             | 1771                                         | 802                                                     |  |  |
| 801                                             | 1772                                         | 803                                                     |  |  |
| 802                                             | 1773                                         | 804                                                     |  |  |
| 803                                             | 1774                                         | 805                                                     |  |  |
| 804                                             | 1775                                         | 806                                                     |  |  |
| 805                                             | 1776                                         | 807                                                     |  |  |
| 806                                             | 1777                                         | 808                                                     |  |  |
| 807                                             | 1778                                         | 809                                                     |  |  |
| 808                                             | 1779                                         | 810                                                     |  |  |
| 809                                             | 1780                                         | 811                                                     |  |  |
| 810                                             | 1781                                         | 812                                                     |  |  |
| 811                                             | 1782                                         | 813                                                     |  |  |
| 812                                             | 1783                                         | 814                                                     |  |  |
| 813                                             | 1784                                         | 815                                                     |  |  |
| 814                                             | 1785                                         | 816                                                     |  |  |
| 815                                             | 1786                                         | 817                                                     |  |  |
| 816                                             | 1787                                         | 818                                                     |  |  |
| 817                                             | 1788                                         | 819                                                     |  |  |
| 818                                             | 1789                                         | 820                                                     |  |  |
| 819                                             | 1790                                         | 821                                                     |  |  |
| 820                                             | 1791                                         | 822                                                     |  |  |
| 821                                             | 1792                                         | 823                                                     |  |  |
| 822                                             | 1793                                         | 824                                                     |  |  |
| 823                                             | 1794                                         | 825                                                     |  |  |
| 824                                             | 1795                                         | 826                                                     |  |  |
| 825                                             | 1796                                         | 827                                                     |  |  |
| 826                                             | 1797                                         | 828                                                     |  |  |
| 827                                             | 1798                                         | 829                                                     |  |  |
| 828                                             | 1799                                         | 830                                                     |  |  |
| 829                                             | 1800                                         | 831                                                     |  |  |
| 830                                             | 1801                                         | 832                                                     |  |  |
| 831                                             | 1802                                         | 833                                                     |  |  |
| 832                                             | 1803                                         | 834                                                     |  |  |
| 833                                             | 1804                                         | 835                                                     |  |  |
| 834                                             | 1805                                         | 836                                                     |  |  |
| 835                                             | 1806                                         | 837                                                     |  |  |
| 836                                             | 1807                                         | 838                                                     |  |  |
| 837                                             | 1808                                         | 839                                                     |  |  |
| 838                                             | 1809                                         | 840                                                     |  |  |
| 839                                             | 1810                                         | 841                                                     |  |  |
| 840                                             | 1811                                         | 842                                                     |  |  |
| 841                                             | 1812                                         | 843                                                     |  |  |
| 842                                             | 1813                                         | 844                                                     |  |  |
| 843                                             | 1814                                         | 845                                                     |  |  |
| 844                                             | 1815                                         |                                                         |  |  |
| 845                                             | 1816                                         | 846                                                     |  |  |
| 846                                             | 1817                                         | 847                                                     |  |  |
| 847                                             |                                              | 848                                                     |  |  |
| 047                                             | 1818                                         | 849                                                     |  |  |

1178 Table 8

| SEQ ID NO of Full-length | Table 8  SEQ ID NO of Full-length   SEQ ID NO in Priority |                             |  |  |  |
|--------------------------|-----------------------------------------------------------|-----------------------------|--|--|--|
| Nucleotide Sequence      | Peptide Sequence                                          | Application USSN 60/324,631 |  |  |  |
| 848                      | 1819                                                      | 850                         |  |  |  |
| 849                      | 1820                                                      | 851                         |  |  |  |
| 850                      | 1821                                                      | 852                         |  |  |  |
| 851                      | 1822                                                      | 853                         |  |  |  |
| 852                      | 1823                                                      | 854                         |  |  |  |
| 853                      | 1824                                                      | 855                         |  |  |  |
| 854                      | 1825                                                      | 856                         |  |  |  |
| 855                      | 1826                                                      | 857                         |  |  |  |
| 856                      | 1827                                                      | 858                         |  |  |  |
| 857                      | 1828                                                      | 859                         |  |  |  |
| 858                      | 1829                                                      | 860                         |  |  |  |
| 859                      | 1830                                                      | 861                         |  |  |  |
| 860                      | 1831                                                      | 862                         |  |  |  |
| 861                      | 1832                                                      | 863                         |  |  |  |
| 862                      | 1833                                                      |                             |  |  |  |
| 863                      | 1834                                                      | 864                         |  |  |  |
| 864                      |                                                           | 865                         |  |  |  |
| 865                      | 1835                                                      | 866                         |  |  |  |
|                          | 1836                                                      | 867                         |  |  |  |
| 866                      | 1837                                                      | 868                         |  |  |  |
| 867                      | 1838                                                      | 869                         |  |  |  |
| 868                      | 1839                                                      | 870                         |  |  |  |
| 869                      | 1840                                                      | 871                         |  |  |  |
| 870                      | 1841                                                      | 872                         |  |  |  |
| 871                      | 1842                                                      | 873                         |  |  |  |
| 872                      | 1843                                                      | 874                         |  |  |  |
| 873                      | 1844                                                      | 875                         |  |  |  |
| 874                      | 1845                                                      | 876                         |  |  |  |
| 875                      | 1846                                                      | 877                         |  |  |  |
| 876                      | 1847                                                      | 878                         |  |  |  |
| 877                      | 1848                                                      | 879                         |  |  |  |
| 878                      | 1849                                                      | 880                         |  |  |  |
| 879                      | 1850                                                      | 881                         |  |  |  |
| 880                      | 1851                                                      | 882                         |  |  |  |
| 881                      | 1852                                                      | 883                         |  |  |  |
| 882                      | 1853                                                      | 884                         |  |  |  |
| 883                      | 1854                                                      | 885                         |  |  |  |
| 884                      | 1855                                                      | 886                         |  |  |  |
| 885                      | 1856                                                      | 887                         |  |  |  |
| 886                      | 1857                                                      | 888                         |  |  |  |
| 887                      | 1858                                                      | 890                         |  |  |  |
| 888                      | 1859                                                      | 891                         |  |  |  |
| 889                      | 1860                                                      | 892                         |  |  |  |
| 890                      | 1861                                                      | 893                         |  |  |  |
| 891                      | 1862                                                      | 894                         |  |  |  |
| 892                      | 1863                                                      | 895                         |  |  |  |
| 893                      | 1864                                                      | 896                         |  |  |  |
| 894                      | 1865                                                      | 897                         |  |  |  |
| 895                      | 1866                                                      |                             |  |  |  |
| 896                      | 1867                                                      | 898                         |  |  |  |
| 897                      | 1868                                                      | 899                         |  |  |  |
| 898                      | 1869                                                      | 900                         |  |  |  |
| 899                      |                                                           | 901                         |  |  |  |
| 900                      | 1870                                                      | 902                         |  |  |  |
| <b>200</b>               | 1871                                                      | 903                         |  |  |  |

1179 Table 8

| SEQ ID NO of Full-length   SEQ ID NO of Full-length   SEQ ID NO in Priority |                  |                             |  |  |
|-----------------------------------------------------------------------------|------------------|-----------------------------|--|--|
| Nucleotide Sequence                                                         | Peptide Sequence | Application USSN 60/324,631 |  |  |
| 901                                                                         | 1872             | 904                         |  |  |
| 902                                                                         | 1873             | 905                         |  |  |
| 903                                                                         | 1874             | 906                         |  |  |
| 904                                                                         | 1875             | 907                         |  |  |
| 905                                                                         | 1876             | 908                         |  |  |
| 906                                                                         | 1877             | 909                         |  |  |
| 907                                                                         | 1878             | 910                         |  |  |
| 908                                                                         | 1879             | 911                         |  |  |
| 909                                                                         | 1880             | 912                         |  |  |
| 910                                                                         | 1881             | 913                         |  |  |
| 911                                                                         | 1882             | 914                         |  |  |
| 912                                                                         | 1883             | 915                         |  |  |
| 913                                                                         | 1884             | 916                         |  |  |
| 914                                                                         | 1885             | 917                         |  |  |
| 915                                                                         | 1886             | 918                         |  |  |
| 916                                                                         | 1887             | 919                         |  |  |
| 917                                                                         | 1888             | 920                         |  |  |
| 918                                                                         | 1889             | 921                         |  |  |
| 919                                                                         | 1890             | 922                         |  |  |
| 920                                                                         | 1891             | 923                         |  |  |
| 921                                                                         | 1892             | 924                         |  |  |
| 922                                                                         | 1893             | 925                         |  |  |
| 923                                                                         | 1894             | 926                         |  |  |
| 924                                                                         | 1895             |                             |  |  |
| 925                                                                         | 1896             | 927                         |  |  |
| 926                                                                         | 1897             | 928                         |  |  |
| 927                                                                         |                  |                             |  |  |
| 928                                                                         | 1898             | 930                         |  |  |
| 929                                                                         | 1000             | 931                         |  |  |
|                                                                             | 1900             | 932                         |  |  |
| 930                                                                         | 1901             | 933                         |  |  |
| 931                                                                         | 1902             | 934                         |  |  |
| 932                                                                         | 1903             | 935                         |  |  |
| 933                                                                         | 1904             | 936                         |  |  |
| 934                                                                         | 1905             | 937                         |  |  |
| 935                                                                         | 1906             | 938                         |  |  |
| 936                                                                         | 1907             | 939                         |  |  |
| 937                                                                         | 1908             | 940                         |  |  |
| 938                                                                         | 1909             | 941                         |  |  |
| 939                                                                         | 1910             | 942                         |  |  |
| 940                                                                         | 1911             | 943                         |  |  |
| 941                                                                         | 1912             | 944                         |  |  |
| 942                                                                         | 1913             | 945                         |  |  |
| 943                                                                         | 1914             | 946                         |  |  |
| 944                                                                         | 1915             | 947                         |  |  |
| 945                                                                         | 1916             | 948                         |  |  |
| 946                                                                         | 1917             | 949                         |  |  |
| 947                                                                         | 1918             | 950                         |  |  |
| 948                                                                         | 1919             | 951                         |  |  |
| 949                                                                         | 1920             | 952                         |  |  |
| 950                                                                         | 1921             | 953                         |  |  |
| 951                                                                         | 1922             | 954                         |  |  |
| 952                                                                         | 1923             | 955                         |  |  |
| 953                                                                         | 1924             | 956                         |  |  |

1180 Table 8

| SEQ ID NO of Full-length<br>Nucleotide Sequence | SEQ ID NO of Full-length<br>Peptide Sequence | SEQ ID NO in Priority Application USSN 60/324,631 |
|-------------------------------------------------|----------------------------------------------|---------------------------------------------------|
| 954                                             | 1925                                         | 957                                               |
| 955                                             | 1926                                         | 958                                               |
| 956                                             | 1927                                         | 959                                               |
| 957                                             | 1928                                         | 960                                               |
| 958                                             | 1929                                         | 961                                               |
| 959                                             | 1930                                         | 962                                               |
| 960                                             | 1931                                         | 963                                               |
| 961                                             | 1932                                         | 964                                               |
| 962                                             | 1933                                         | 965                                               |
| 963                                             | 1934                                         | 966                                               |
| 964                                             | 1935                                         | 967                                               |
| 965                                             | 1936                                         | 968                                               |
| 966                                             | 1937                                         | 969                                               |
| 967                                             | 1938                                         | 970                                               |
| 968                                             | 1939                                         | 971                                               |
| 969                                             | 1940                                         | 972                                               |
| 970                                             | 1941                                         | 973                                               |
| 971                                             | 1942                                         | 974                                               |

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## WHAT IS CLAIMED IS:

- 1. An isolated polynucleotide comprising a nucleotide sequence selected from the group consisting of SEQ ID NO: 1-971.
- 2. An isolated polynucleotide encoding a polypeptide with biological activity, wherein said polynucleotide hybridizes to the polynucleotide of claim 1 under stringent hybridization conditions.
- 3. An isolated polynucleotide encoding a polypeptide with biological activity, wherein said polynucleotide has greater than about 99% sequence identity with the polynucleotide of claim 1.
- 4. The polynucleotide of claim 1 wherein said polynucleotide is DNA.
- 5. An isolated polynucleotide of claim 1 wherein said polynucleotide comprises the complementary sequences.
- 6. A vector comprising the polynucleotide of claim 1.
- 7. An expression vector comprising the polynucleotide of claim 1.
- 8. A host cell genetically engineered to comprise the polynucleotide of claim 1.
- 9. A host cell genetically engineered to comprise the polynucleotide of claim 1 operatively associated with a regulatory sequence that modulates expression of the polynucleotide in the host cell.
- 10. An isolated polypeptide, wherein the polypeptide is selected from the group consisting of:
  - (a) a polypeptide encoded by any one of the polynucleotides of claim 1; and
  - (b) a polypeptide encoded by a polynucleotide hybridizing under stringent conditions with any one of SEQ ID NO: 1-971.

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- 11. A composition comprising the polypeptide of claim 10 and a carrier.
- 12. An antibody directed against the polypeptide of claim 10.
- 13. A method for detecting the polynucleotide of claim 1 in a sample, comprising:
- a) contacting the sample with a compound that binds to and forms a complex with the polynucleotide of claim 1 for a period sufficient to form the complex; and
- b) detecting the complex, so that if a complex is detected, the polynucleotide of claim 1 is detected.
- 14. A method for detecting the polynucleotide of claim 1 in a sample, comprising:
- a) contacting the sample under stringent hybridization conditions with nucleic acid primers that anneal to the polynucleotide of claim 1 under such conditions;
- b) amplifying a product comprising at least a portion of the polynucleotide of claim 1; and
- c) detecting said product and thereby the polynucleotide of claim 1 in the sample.
- 15. The method of claim 14, wherein the polynucleotide is an RNA molecule and the method further comprises reverse transcribing an annealed RNA molecule into a cDNA polynucleotide.
- 16. A method for detecting the polypeptide of claim 10 in a sample, comprising:
- a) contacting the sample with a compound that binds to and forms a complex with the polypeptide under conditions and for a period sufficient to form the complex; and
- b) detecting formation of the complex, so that if a complex formation is detected, the polypeptide of claim 10 is detected.
- 17. A method for identifying a compound that binds to the polypeptide of claim 10, comprising:

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- a) contacting the compound with the polypeptide of claim 10 under conditions sufficient to form a polypeptide/compound complex; and
- b) detecting the complex, so that if the polypeptide/compound complex is detected, a compound that binds to the polypeptide of claim 10 is identified.
- 18. A method for identifying a compound that binds to the polypeptide of claim 10, comprising:
- a) contacting the compound with the polypeptide of claim 10, in a cell, under conditions sufficient to form a polypeptide/compound complex, wherein the complex drives expression of a reporter gene sequence in the cell; and
- b) detecting the complex by detecting reporter gene sequence expression, so that if the polypeptide/compound complex is detected, a compound that binds to the polypeptide of claim 10 is identified.
- 19. A method of producing the polypeptide of claim 10, comprising,
- a) culturing a host cell comprising a polynucleotide sequence selected from the group consisting of any of the polynucleotides from SEQ ID NO: 1-971, under conditions sufficient to express the polypeptide in said cell; and
  - b) isolating the polypeptide from the cell culture or cells of step (a).
- 20. An isolated polypeptide comprising an amino acid sequence selected from the group consisting of any one of the polypeptides SEQ ID NO: 972-1942.
- 21. The polypeptide of claim 20 wherein the polypeptide is provided on a polypeptide array.
- 22. A collection of polynucleotides, wherein the collection comprising of at least one of SEQ ID NO: 1-971.
- 23. The collection of claim 22, wherein the collection is provided on a nucleic acid array.
- 24. The collection of claim 23, wherein the array detects full-matches to any one of the polynucleotides in the collection.

25. The collection of claim 23, wherein the array detects mismatches to any one of the polynucleotides in the collection.

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26. The collection of claim 22, wherein the collection is provided in a computer-readable format.